

Supplementary Information

Molecular conformational effects on the overall rate constant and the branching ratios of the *n*-heptane + OH reaction: An *ab initio* and variational transition state theory study

M. Belmekki, M. Monge-Palacios*, T. Wang and S. M. Sarathy

King Abdullah University of Science and Technology (KAUST), Physical Sciences and Engineering Division, Clean Energy Research Platform (CERP), Thuwal (Makkah), 23955-6900, Saudi Arabia

*E-mail: manuel.mongepalacios@kaust.edu.sa

Table S1. Optimized Cartesian coordinates matrix and vibrational frequencies of all the conformers of the <i>n</i> -heptane and the saddle point species involved in reactions R1-R4 at the M06-2X/aug-cc-pVTZ level of theory	2
Table S2. Computed energies of all the conformers of the stationary points involved in reactions R1-R4 at the M06-2X/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ levels of theory with their associated T1 diagnostic values provided for the conformers whose energy is below 1 kcal mol ⁻¹ of the corresponding global minimum.....	65
Table S3. Site-specific rate constants obtained with the SS-HO-LL approach	68
Table S4. Site-specific rate constants obtained with the SS-HO-HL approach	68
Table S5. Site-specific rate constants obtained with the MS-T-HL approach.....	69
Table S6. Site-specific rate constants obtained with the MS-T-HL_0.5 approach.....	69
Table S7. Site-specific rate constants obtained with the MS-T-HL_1.0 approach.....	70

Table S1. Optimized Cartesian coordinates matrix and vibrational frequencies of all the conformers of the n-heptane and the saddle point species involved in reactions R1-R4 at the M06-2X/aug-cc-pVTZ level of theory

Conformer species	Geometry (Å)			Frequencies (cm ⁻¹)	
n-heptane_1	C	-3.80717178	-0.35596736	-0.00000004	65.6113, 73.9494, 100.1713, 144.1797, 145.0937, 244.7554, 247.2133, 248.5124, 306.9299, 421.9920, 487.8794, 727.1549, 734.9753, 773.3901, 849.6397, 896.2361, 927.4946, 942.7722, 1020.7411, 1030.9346, 1062.2940, 1087.6354, 1089.9824, 1101.1320, 207.3254, 1243.9078, 1257.8138, 1295.1243, 1317.2535, 1326.3293, 1333.9146, 1339.9993, 1369.9234, 1403.8659, 1409.7655, 1413.2859, 1416.1307, 1485.4881, 1485.6073, 1491.1407, 1496.6661, 1502.8408, 1502.9107, 1504.3303, 1511.5837, 1515.5993, 3028.4736, 3029.9720, 3037.6233, 3047.8111, 3049.77073056.5932, 3056.8965, 3059.0592, 3072.7528, 3085.1919, 3092.9886, 3122.6583, 3122.8757, 3131.5038, 3131.6150
	H	-3.83984778	-0.99962975	0.88025638	
	H	-4.70763972	0.25731720	-0.00000039	
	H	-3.83984739	-0.99962905	-0.88025687	
	C	-1.27203629	-0.34116738	0.00000022	
	H	-1.27303627	-0.99879095	0.87509225	
	H	-1.27303581	-0.99879070	-0.87509304	
	C	-2.54473496	0.49607013	0.00000017	
	H	-2.54181512	1.15188818	-0.87449573	
	H	-2.54181555	1.15188750	0.87449661	
	C	0.00000007	0.49619283	-0.00000017	
	H	0.00000003	1.15355751	0.87515911	
	H	0.00000061	1.15355775	-0.87515828	
	C	1.27203599	-0.34116781	-0.00000035	
	H	1.27303621	-0.99879062	-0.87509256	
	H	1.27303672	-0.99879111	0.87509273	
	C	2.54473467	0.49607028	-0.00000005	
H	2.54181553	1.15188795	-0.87449600		
H	2.54181607	1.15188702	0.87449634		
C	3.80717176	-0.35596714	0.00000014		
H	3.83984761	-0.99962895	-0.88025648		
H	3.83984809	-0.99963029	0.88025585		
H	4.70763992	0.25731702	0.00000056		
n-heptane_2	C	-3.70206678	0.03360892	0.14566506	47.0855, 79.3152, 115.4298, 134.4324, 146.8374, 244.2441, 245.6840, 288.1332, 358.1335, 396.8340, 496.3620, 724.9348, 744.6567, 778.9186, 842.6708, 884.1732, 919.4076, 946.2947, 984.5953, 1031.7831, 1052.3778, 1082.7736, 1096.8329, 1107.7901, 97.7445, 1238.5393, 1261.3813, 1294.9541, 1311.0794, 1332.2872, 1335.2544, 1348.3553, 1379.2223, 1396.0043, 1409.1335, 1413.0634, 1416.2128, 1482.9391, 1485.9044, 1492.7377, 1494.1798, 1502.8995, 1504.2995, 1505.9000, 1513.2008, 1513.7994, 3028.5903, 3031.6269, 3040.5681, 3047.9885, 3048.8224, 057.4290, 3058.5557, 3068.1375, 3080.9940, 3086.3566, 3095.5787, 3123.4728, 3124.9158, 3131.3694, 3134.8457
	H	-3.76825414	-0.13371177	1.22169493	
	H	-4.49018362	0.73204320	-0.13367241	
	H	-3.90593248	-0.91722124	-0.34885299	
	C	-1.20489821	-0.40375911	0.14592053	
	H	-1.23981388	-0.58708036	1.22466203	
	H	-1.38144613	-1.37192875	-0.33326839	
	C	-2.32363908	0.55699701	-0.23613908	
	H	-2.28419406	0.74229367	-1.31271074	
	H	-2.14814933	1.52150452	0.24729677	
	C	0.18066186	0.10250879	-0.23377981	
	H	0.34099324	1.07773628	0.23312507	
	H	0.22229641	0.26850344	-1.31557315	
	C	1.29384708	-0.85743400	0.17065985	
	H	1.06296520	-1.85028650	-0.22456040	
	H	1.30294699	-0.95489138	1.26101194	
	C	2.68179833	-0.43853249	-0.30792530	
H	3.40019839	-1.21347020	-0.03386629		
H	2.68339556	-0.38914946	-1.40011286		
C	3.14364500	0.89819974	0.26208417		
H	3.09439470	0.89025095	1.35264798		
H	2.52264950	1.72047993	-0.09214148		
H	4.17204450	1.11539448	-0.02459255		
n-heptane_3	C	-3.44430417	-0.79948929	0.10576099	65.0924, 72.5589, 97.5627, 125.6634, 206.3189, 240.8220, 247.3269, 273.8433, 311.4975, 407.2219, 516.3271, 726.5126, 743.7327, 783.6639, 853.3271, 869.9121,
	H	-3.42381828	-1.06287364	1.16429455	
	H	-4.46428919	-0.51289212	-0.14820609	
	H	-3.19718844	-1.69754862	-0.46220777	
	C	-1.02012608	-0.05755806	0.16098046	
	H	-0.96274304	-0.30510879	1.22647083	

	H	-0.75043317	-0.96818751	-0.38037435	917.6691, 943.3285, 987.4851,
	C	-2.45387462	0.31851463	-0.19200861	1039.6484, 1057.3761, 1072.9004,
	H	-2.50327340	0.58315407	-1.25156174	1093.9838, 1110.6257, 16.4077,
	H	-2.73489799	1.21820384	0.36145594	1244.1191, 1270.6435, 1295.5201,
	C	-0.02195738	1.05122484	-0.15328133	1310.1215, 1331.2696, 1333.1307,
	H	-0.37009328	1.97848121	0.30963498	1344.0412, 1377.0407, 1404.5499,
	H	-0.01588635	1.23095049	-1.23303702	1409.2702, 1412.9435, 1414.0568,
	C	1.40081196	0.76172699	0.31677424	1483.7817, 1488.3713, 1491.1690,
	H	1.40335496	0.63076516	1.40367673	1497.6578, 1501.7328, 1503.8073,
	H	2.03042376	1.63189760	0.11195093	1504.1161, 1511.8436, 1513.8903,
	C	2.03544445	-0.46376046	-0.33229310	3029.4819, 3033.9362, 3037.4414,
	H	1.47562129	-1.35948549	-0.05689197	3048.5126, 3048.7529, 56.6987,
	H	1.95783078	-0.37282240	-1.41955431	3061.2032, 3068.1302, 3075.6011,
	C	3.49478125	-0.63760200	0.06850372	3092.1872, 3095.2350, 3123.0884,
	H	3.58819432	-0.74130358	1.15063073	3123.7071, 3130.3830, 3130.5325
	H	4.08544885	0.22912475	-0.23149878	
	H	3.93709671	-1.52069490	-0.39140085	
n-heptane_4	C	3.24721687	0.64185011	0.31226485	
	H	3.39930497	0.22684477	1.30972303	64.7107, 77.8751, 132.2236, 147.7734,
	H	4.20686703	0.63382211	-0.20347235	199.9727, 247.8050, 277.3762,
	H	2.93931292	1.68166416	0.43135055	294.3330, 383.0127, 403.8290,
	C	0.84150485	-0.15814356	0.25737725	505.1098, 721.1709, 743.2936,
	H	0.95629152	-0.59028894	1.25735613	798.8855, 850.7434, 857.6947,
	H	0.51601536	0.87550333	0.40778182	919.2589, 948.4735, 970.1991,
	C	2.19213138	-0.15104416	-0.44774056	1031.4239, 1041.1580, 1072.4929,
	H	2.06871114	0.26526207	-1.45108322	1093.5106, 1118.14781177.3204,
	H	2.53086083	-1.18131323	-0.58358476	1239.6951, 1261.3565, 1297.2607,
	C	-0.22441835	-0.93183136	-0.50920799	1303.0743, 1330.3378, 1333.1082,
	H	0.15863038	-1.92955166	-0.73891895	1364.3170, 1384.6608, 1389.9630,
	H	-0.39516352	-0.44587197	-1.47380641	1409.6004, 1412.6517, 1414.5849,
	C	-1.54694289	-1.07430860	0.24282359	1480.7400, 1488.8399, 1494.4246,
	H	-1.38389807	-1.68970404	1.13151666	1497.1008, 1500.7112, 1503.3326,
	H	-2.25502239	-1.61983452	-0.38679678	1506.4381, 1511.2113, 1518.3779,
	C	-2.18329211	0.24960723	0.66633869	3028.9931, 3041.2834, 3045.0479,
H	-3.13174526	0.03688385	1.16296075	3050.1899, 3056.073 3057.1073,	
H	-1.55392612	0.73892823	1.41277793	3062.0593, 3074.2437, 3081.6093,	
C	-2.42496640	1.20104759	-0.49974515	3092.8243, 3094.4128, 3122.2639,	
H	-3.00771117	0.71323783	-1.28349769	3122.7416, 3131.6055, 3132.0043	
H	-1.48633618	1.53269618	-0.94505643		
H	-2.96959155	2.08865843	-0.17991434		
n-heptane_5	C	2.99284646	-1.00761485	0.04453158	60.2815, 77.3173, 110.5551, 205.6794,
	H	2.76704767	-1.55812910	0.95915872	206.8901, 246.0914, 256.7272,
	H	3.39229434	-1.71482727	-0.68159535	295.9645, 311.1036, 428.0080,
	H	3.77775855	-0.28725393	0.27908811	527.3812, 719.4038, 748.4702,
	C	1.17035443	0.67877804	0.53351353	792.5087, 847.6506, 881.6313,
	H	0.86289711	0.12878351	1.42735021	892.9018, 945.7228, 969.8501,
	H	1.96214572	1.35947387	0.85746644	1050.0761, 1057.2274, 1065.9666,
	C	1.74900935	-0.30197777	-0.48005560	1072.3733, 1122.3648, 75.6155,
	H	1.98705149	0.23420921	-1.40327363	1248.5847, 1257.0754, 1304.5951,
	H	0.99478420	-1.04695332	-0.74444697	1313.3061, 1328.9230, 1331.1732,
	C	-0.00000002	1.50374327	0.00000003	1346.4605, 1391.0897, 1399.5763,
	H	0.36377246	2.15835482	-0.79640313	1409.9597, 1411.5140, 1412.9115,
	H	-0.36377249	2.15835477	0.79640322	1483.7607, 1490.4613, 1493.9124,
	C	-1.17035449	0.67877811	-0.53351349	1496.9686, 1502.3699, 1503.5683,
	H	-0.86289722	0.12878371	-1.42735028	1503.5929, 1509.8923, 1515.3060,
	H	-1.96214582	1.35947397	-0.85746626	3038.0906, 3039.4417, 3044.1310,
	C	-1.74900929	-0.30197786	0.48005555	3049.5615, 3049.8013, 056.2222,
H	-0.99478410	-1.04695343	0.74444673		

	H	-1.98705132	0.23420899	1.40327369	3066.3777, 3068.3110, 3080.1952,
	C	-2.99284645	-1.00761486	-0.04453159	3091.7589, 3092.4434, 3121.7510,
	H	-2.76704779	-1.55812890	-0.95915889	3122.1742, 3130.7479, 3130.7715
	H	-3.77775860	-0.28725392	-0.27908783	
	H	-3.39229419	-1.71482746	0.68159524	
n-heptane_6	C	-3.02418020	-0.74939224	0.04408302	65.4155, 103.3952, 115.0676,
	H	-2.70793284	-1.74507665	-0.27088409	187.9863, 217.3812, 253.8141,
	H	-3.70583193	-0.86569503	0.88596436	286.6980, 314.6354, 362.5041,
	H	-3.58204186	-0.30467799	-0.78120628	433.1833, 533.9501, 715.1465,
	C	-0.85089388	0.26886480	-0.75916986	748.9184, 795.1387, 841.1077,
	H	-0.46802036	-0.71647606	-1.04224343	878.4015, 891.8342, 949.6037,
	H	-1.40358621	0.63718473	-1.62756236	961.6522, 1028.7779, 1054.3296,
	C	-1.81913565	0.10844696	0.40768672	1061.3612, 1073.4736,
	H	-2.15220671	1.09740476	0.73538826	1124.5016, 169.9569, 1236.6082,
	H	-1.30035019	-0.33787058	1.25907093	1253.8729, 1293.4377, 1316.5696,
	C	0.31113112	1.21819600	-0.47404538	1324.5487, 1338.4620, 1367.4433,
	H	-0.08571518	2.22297252	-0.30729275	1384.6381, 1397.4540, 1408.5080,
	H	0.94326934	1.28533504	-1.36212346	1411.6154, 1415.9843, 1479.2889,
	C	1.16752511	0.82545738	0.73193189	1490.8563, 1494.0291, 1500.4826,
	H	0.58667987	0.95176504	1.64812024	1502.2589, 1503.2430, 1507.1153,
	H	2.00675105	1.52230109	0.80468734	1513.3679, 1516.8938, 3038.6920,
	C	1.71409422	-0.60052804	0.67869702	3045.4849, 3049.2321, 3052.4374,
H	2.31561485	-0.77808764	1.57206886	3055.75983058.3740, 3069.6416,	
H	0.88792666	-1.31466698	0.72320261	3078.5271, 3087.4090, 3092.3400,	
C	2.55740399	-0.87516450	-0.56131254	3097.4477, 3122.8005, 3123.8017,	
H	3.36351331	-0.14436761	-0.64993281	3130.9209, 3132.6590	
H	1.95954591	-0.81845241	-1.47137232		
H	3.00671606	-1.86687440	-0.52311033		
n-heptane_7	C	2.79323884	0.47293152	-0.08496967	84.3264, 86.9908, 128.6339, 201.7410,
	H	3.31996395	-0.05702593	0.71093243	208.3462, 262.1307, 323.6467,
	H	3.53271620	0.80571252	-0.81247628	337.5779, 388.3613, 441.7668,
	H	2.33950168	1.36168384	0.35438822	535.2482, 710.4454, 750.4495,
	C	0.76570116	-1.03043784	0.27282297	804.6088, 833.3652, 879.6026,
	H	0.05640943	-1.66876952	-0.26004144	886.8108, 951.7796, 963.6982,
	H	1.31657792	-1.68719431	0.95134293	1004.3447, 1050.9097, 1057.2076,
	C	1.74631010	-0.42658897	-0.73221940	1077.1609, 1119.0662, 71.0941,
	H	1.19829857	0.13949773	-1.48934835	1222.3371, 1248.9535, 1291.4611,
	H	2.24590344	-1.23852580	-1.26389281	1306.4067, 1332.8028, 1355.7753,
	C	0.00000000	0.00000001	1.10407580	1373.1197, 1380.0933, 1400.1539,
	H	0.69421175	0.52568307	1.76306451	1401.1038, 1414.1831, 1416.4248,
	H	-0.69421177	-0.52568303	1.76306451	1478.0253, 1487.4772, 1496.4249,
	C	-0.76570117	1.03043786	0.27282295	1500.1015, 1501.1665, 1504.6633,
	H	-0.05640944	1.66876953	-0.26004147	1512.2210, 1513.1102, 1521.5783,
	H	-1.31657794	1.68719434	0.95134291	3045.0523, 3046.9046, 3052.1358,
	C	-1.74631011	0.42658896	-0.73221941	3054.6319, 3057.4078, 062.5229,
H	-2.24590345	1.23852577	-1.26389284	3077.4040, 3081.7150, 3088.3930,	
H	-1.19829856	-0.13949774	-1.48934835	3094.1978, 3096.8158, 3123.1692,	
C	-2.79323882	-0.47293154	-0.08496966	3123.2233, 3131.7200, 3131.9324	
H	-3.31996391	0.05702590	0.71093246		
H	-2.33950164	-1.36168386	0.35438820		
H	-3.53271621	-0.80571253	-0.81247625		
n-heptane_8	C	-2.65408176	0.95715544	0.33038823	45.7002, 82.9846, 139.3326, 168.5655,
	H	-2.21109508	1.81619916	-0.17779926	228.8863, 252.4399, 290.3701,
	H	-3.73099182	1.11513138	0.37732873	304.8146, 356.2635, 442.2512,
	H	-2.27773224	0.94658111	1.35288858	521.9545, 722.6030, 765.5719,
	C	-0.81653462	-0.52976326	-0.62082945	796.3330, 844.4369, 852.6081,
	H	-0.64905889	-1.43754582	-1.20798910	907.1586, 949.0614, 966.2624,
H	-0.43818638	0.30087357	-1.22444787		

	C	-2.31524563	-0.33563510	-0.40405765	1011.2153, 1045.7974, 1068.4446,
	H	-2.71075492	-1.18759266	0.15536967	1093.0841, 1120.9785, 69.4539,
	H	-2.81854926	-0.34165345	-1.37274006	1231.8203, 1261.0905, 1295.8917,
	C	-0.01817111	-0.62715281	0.67550462	1313.5599, 1326.1112, 1343.0434,
	H	-0.49382444	-1.36331477	1.32999201	1376.2238, 1378.2257, 1389.3914,
	H	-0.06163921	0.32471892	1.20898638	1408.1144, 1414.3428, 1416.3499,
	C	1.44204077	-1.02337481	0.46140617	1479.5120, 1491.5603, 1493.2893,
	H	1.47930534	-2.03851513	0.05739920	1496.6515, 1500.5248, 1504.0821,
	H	1.94677921	-1.05531722	1.43071355	1508.7126, 1512.5735, 1518.4119,
	C	2.21876820	-0.09011258	-0.46787752	3035.0203, 3041.7608, 3047.8283,
	H	3.25233722	-0.43632136	-0.52541358	3049.9320, 3055.2738, 060.0481,
	H	1.81837181	-0.16247410	-1.48138417	3069.6764, 3077.8544, 3086.1585,
	C	2.19684847	1.36513945	-0.01438120	3093.0589, 3099.2322, 3122.1347,
	H	2.54151351	1.45487481	1.01760497	3123.7347, 3130.4805, 3136.3577
	H	1.19057009	1.78329646	-0.06321154	
	H	2.84120911	1.98352113	-0.63821665	
n-heptane_9	C	3.49142583	-0.37396817	0.04537676	50.6747, 79.2780, 116.6661, 131.1930,
	H	3.75320262	0.22182989	0.92114457	235.5808, 237.6986, 266.3067,
	H	3.99463902	-1.33629120	0.13301007	288.7343, 307.9119, 415.2727,
	H	3.89214433	0.13612335	-0.83174998	538.0276, 732.9040, 757.0375,
	C	1.26308514	0.80602936	-0.17328217	784.7206, 842.0819, 867.4427,
	H	1.44322624	1.38135645	0.74054810	903.2473, 949.8096, 965.3166,
	H	1.71113278	1.37863340	-0.98993751	1038.9425, 1050.6038, 1070.4810,
	C	1.98070884	-0.53516505	-0.06455028	1089.5629, 1117.7124, 15.0595,
	H	1.73514791	-1.14385424	-0.93959978	1239.3231, 1268.3487, 1304.6432,
	H	1.61023935	-1.08164910	0.80488993	1307.3544, 1327.3083, 1335.3805,
	C	-0.24038938	0.68758343	-0.40792245	1351.3917, 1378.9202, 1402.3834,
	H	-0.41091751	0.16788352	-1.35455966	1405.4015, 1412.5298, 1416.1492,
	H	-0.66661203	1.68851424	-0.52419646	1480.8632, 1488.5412, 1493.8863,
	C	-0.98050979	-0.03355159	0.71603724	1497.3774, 1500.7379, 1503.7599,
	H	-0.64887217	0.37499817	1.67527719	1505.8392, 1512.1298, 1512.8604,
	H	-0.70555728	-1.09181186	0.71891445	3031.4100, 3035.7552, 3043.0994,
	C	-2.49981839	0.08127137	0.61822950	3047.6198, 3048.0801, 57.8936,
	H	-2.95065046	-0.40935479	1.48297438	3065.7907, 3068.0665, 3083.3937,
	H	-2.78339558	1.13548114	0.67794660	3092.7621, 3094.8031, 3122.9691,
	C	-3.06935893	-0.52633050	-0.65904714	3124.8279, 3131.6255, 3135.5969
	H	-2.75144938	-1.56514961	-0.76703760	
	H	-2.73448570	0.01646227	-1.54266253	
	H	-4.15865210	-0.50838477	-0.65401052	
n-heptane_10	C	2.91067974	-0.89965447	-0.51846370	48.2400, 91.4131, 116.9476, 126.6666,
	H	3.03676668	-0.39096143	-1.47614336	168.2196, 252.6260, 287.9750,
	H	3.85391289	-1.38543884	-0.27092934	306.6482, 319.9441, 460.0912,
	H	2.16348359	-1.68113552	-0.65380066	469.9867, 731.9560, 749.2044,
	C	1.24983818	0.89454222	0.21004326	787.3917, 841.4015, 877.5642,
	H	1.05231636	1.61978962	1.00410512	907.2817, 953.7112, 970.4970,
	H	1.44345722	1.47661653	-0.69663243	1019.4530, 1036.4392, 1082.4694,
	C	2.49656656	0.08873848	0.56621994	1102.1714, 1110.1090, 88.0474,
	H	2.31946275	-0.44936901	1.50130067	1232.5070, 1264.8701, 1301.5342,
	H	3.32124258	0.77757536	0.75903153	1306.0281, 1329.8955, 1334.0907,
	C	-0.00000002	0.04647856	-0.00000004	1377.9960, 1378.3464, 1381.9250,
	H	-0.13296105	-0.60826971	0.86606261	1407.4238, 1415.7215, 1415.8932,
	H	0.13296100	-0.60826959	-0.86606277	1481.6847, 1485.7356, 1493.3799,
	C	-1.24983822	0.89454225	-0.21004321	1493.7380, 1504.1293, 1504.9782,
	H	-1.05231645	1.61978973	-1.00410502	1507.5340, 1512.9179, 1512.9400,
	H	-1.44345724	1.47661647	0.69663254	3032.3849, 3033.1675, 3043.3610,
	C	-2.49656660	0.08873853	-0.56621990	3047.0992, 3048.2344, 058.3979,
	H	-3.32124267	0.77757541	-0.75903135	3062.7907, 3074.0095, 3084.0218,
	H	-2.31946283	-0.44936884	-1.50130071	

	C	-2.91067965	-0.89965457	0.51846365	3086.9087, 3095.3267, 3124.8111,
	H	-3.03676655	-0.39096164	1.47614338	3124.8704, 3134.9030, 3134.9174
	H	-2.16348342	-1.68113558	0.65380047	
	H	-3.85391278	-1.38543896	0.27092931	
n-heptane_11	C	2.77990735	1.15698942	0.10924149	46.1992, 79.7507, 103.5237, 140.3448,
	H	2.73530754	1.27326453	1.19378980	159.3452, 254.2583, 270.1238,
	H	3.75375320	1.51281550	-0.22542877	310.9461, 326.1643, 462.1947,
	H	2.02413274	1.81018892	-0.32585308	463.2305, 730.2555, 767.3079,
	C	1.26796319	-0.89371899	0.27262153	776.8507, 835.9782, 882.4899,
	H	1.21949318	-1.95404234	0.01090325	907.8160, 953.6946, 973.3874,
	H	1.29436770	-0.84786761	1.36619345	1019.1309, 1038.7273, 1082.9618,
	C	2.55836022	-0.29895734	-0.28616570	1100.5513, 1110.3117, 194.3378,
	H	2.54813142	-0.38334107	-1.37617192	1228.9870, 1265.0915, 1293.6120,
	H	3.40298796	-0.89733212	0.06069932	1319.9833, 1324.8041, 1335.9378,
	C	-0.00000000	-0.20686493	-0.22286553	1375.1363, 1379.3745, 1384.5679,
	H	-0.00000000	-0.19397269	-1.31867511	1408.6203, 1414.8814, 1416.2512,
	H	0.00000000	0.83603352	0.09923635	1482.2678, 1486.5539, 1492.5544,
	C	-1.26796320	-0.89371900	0.27262153	1493.1553, 1504.4326, 1504.5929,
	H	-1.29436771	-0.84786763	1.36619345	1507.7093, 1511.6399, 1512.5271,
	H	-1.21949319	-1.95404234	0.01090323	3027.4294, 3033.6909, 3041.9898,
	C	-2.55836023	-0.29895734	-0.28616569	3047.9896, 3048.4212, 3058.6511,
	H	-2.54813145	-0.38334107	-1.37617191	3070.8759, 3074.8946, 3085.2088,
	H	-3.40298797	-0.89733210	0.06069934	3086.5990, 3102.9917, 3124.8988,
	C	-2.77990734	1.15698943	0.10924148	3125.3563, 3134.3096, 3135.8830
	H	-2.02413272	1.81018892	-0.32585310	
	H	-2.73530750	1.27326455	1.19378980	
	H	-3.75375319	1.51281552	-0.22542875	
n-heptane_12	C	3.57139086	-0.13048493	0.16675540	30.4738, 72.1182, 103.5754, 124.5508,
	H	3.65645452	0.09686631	1.23050546	222.9483, 239.3816, 263.3539,
	H	4.21837770	-0.98080319	-0.04620570	286.1815, 299.5320, 414.3094,
	H	3.95356032	0.72928285	-0.38537596	530.8903, 726.1077, 743.9291,
	C	1.20517597	0.76240420	0.10044639	782.3816, 850.2523, 867.5151,
	H	1.20488242	0.94018810	1.18074540	902.6125, 950.0972, 966.8642,
	H	1.62748349	1.66153651	-0.35654899	1041.7802, 1045.5941, 1072.7502,
	C	2.12287756	-0.41578861	-0.20916661	1088.2976, 1117.3236, 193.4718,
	H	2.05617469	-0.65030445	-1.27542761	1234.9542, 1271.8444, 1292.6572,
	H	1.78058661	-1.30427266	0.32423539	1314.7523, 1328.2832, 1340.0784,
	C	-0.23290120	0.58708529	-0.38206668	1351.9034, 1379.5570, 1401.3690,
	H	-0.23411461	0.43500437	-1.46668248	1408.1372, 1413.4574, 1416.1314,
	H	-0.77688456	1.51583458	-0.20021347	1481.8705, 1486.5149, 1492.1121,
	C	-0.97076677	-0.57125683	0.28195481	1497.1522, 1500.1886, 1503.8852,
	H	-0.95429413	-0.42928271	1.36802522	1505.0572, 1512.1180, 1512.2728,
	H	-0.43710063	-1.50257497	0.08357577	3029.1494, 3032.4217, 3039.7655,
	C	-2.41747924	-0.72847514	-0.18286623	3049.1343, 3049.9098, 3058.8997,
	H	-2.43005486	-0.87801585	-1.26591769	3067.3929, 3078.9882, 3085.9291,
	H	-2.83220329	-1.63740333	0.25709822	3094.0436, 3101.6390, 3124.0997,
	C	-3.31185320	0.45246559	0.17907127	3125.5542, 3130.5509, 3135.4858
	H	-3.01079856	1.36141511	-0.34051370	
	H	-3.27023672	0.65288774	1.25132136	
	H	-4.35049634	0.25394420	-0.08339138	
n-heptane_13	C	3.15372559	0.24429929	-0.22021536	38.2292, 77.4308, 123.4049, 172.5326,
	H	3.29946578	0.92711731	0.61891239	222.7190, 250.0980, 291.6882,
	H	4.11697676	-0.20813206	-0.45368647	296.0979, 357.2535, 435.9524,
	H	2.85268263	0.83759855	-1.08284549	516.8753, 720.1570, 749.4141,
	C	0.77886347	-0.24484822	0.59086949	797.0698, 848.1419, 856.5827,
	H	0.14090569	-1.06872542	0.91900613	905.0603, 955.9748, 960.6134,
	H	0.94278575	0.38701202	1.47062330	1012.2792, 1044.1083, 1070.7926,
	C	2.11563559	-0.81818282	0.12441481	

	H	1.94469803	-1.45784776	-0.74585957	1095.2473, 1120.9594, 177.6181,
	H	2.51441192	-1.46577134	0.90756542	1229.1559, 1261.8979, 1296.8049,
	C	0.04936358	0.56389085	-0.47633650	1306.9557, 1333.6219, 1341.3457,
	H	-0.12327319	-0.07223965	-1.34959287	1377.5521, 1379.7206, 1389.6674,
	H	0.68804862	1.38034334	-0.81811274	1409.2643, 1414.3591, 1416.1754,
	C	-1.27425697	1.16033280	0.00287725	1479.6720, 1489.6118, 1493.1039,
	H	-1.73145544	1.70966180	-0.82453229	1496.7436, 1500.7798, 1504.1194,
	H	-1.06813054	1.89502252	0.78577809	1507.8028, 1512.3787, 1517.9016,
	C	-2.28419100	0.14152459	0.53177228	3030.3857, 3041.7272, 3046.1548,
	H	-1.91365128	-0.30165569	1.45838725	3049.0191, 3056.05023060.2874,
	H	-3.20252834	0.66895036	0.79637658	3075.9628, 3078.4483, 3085.2608,
	C	-2.60531010	-0.96249944	-0.46889345	3094.0911, 3098.9575, 3122.4307,
	H	-1.73566669	-1.59183028	-0.66138932	3125.4715, 3131.1580, 3137.0038
	H	-2.92408103	-0.53955949	-1.42355737	
	H	-3.40416965	-1.60704654	-0.10400413	
n-heptane_14	C	2.98024302	-1.04415173	0.11716611	61.7372, 96.6732, 133.6846, 147.7377,
	H	3.19123350	-0.92613179	1.18113745	217.0997, 247.6164, 250.4687,
	H	3.11193358	-2.09567739	-0.13555365	284.5340, 319.2497, 425.6016,
	H	3.72767480	-0.47025019	-0.43246647	497.9634, 731.1483, 750.8130,
	C	1.37673341	0.91001477	0.15360354	795.6597, 857.8452, 876.8204,
	H	1.52258141	1.02550031	1.23248116	892.9013, 950.0535, 977.1508,
	H	2.16315250	1.49987997	-0.32557901	1042.7988, 1064.2696, 1075.9805,
	C	1.57462519	-0.55676797	-0.21086173	1081.4647, 1117.5754, 86.2306,
	H	1.37304990	-0.69505223	-1.27689448	1244.8809, 1262.4511, 1289.0098,
	H	0.84506483	-1.16944644	0.32393598	1323.5793, 1330.8601, 1336.0384,
	C	0.01540062	1.49052369	-0.22685789	1337.5018, 1380.7615, 1397.6656,
	H	-0.09292513	1.47176139	-1.31582772	1407.2938, 1411.5106, 1412.5421,
	H	0.00322607	2.54279976	0.06117428	1484.1667, 1491.3238, 1496.5858,
	C	-1.17956992	0.76644722	0.40830214	1498.7051, 1499.4841, 1502.8293,
	H	-1.94954897	1.49081102	0.68406059	1504.0684, 1511.3389, 1516.3646,
	H	-0.86335286	0.29419483	1.34459911	3032.1341, 3032.4490, 3041.0805,
	C	-1.82379302	-0.28389391	-0.49311155	3046.6587, 3053.8015, 056.8834,
	H	-2.20922937	0.21285655	-1.38717479	3064.7945, 3072.2131, 3087.4024,
	H	-1.06804282	-0.99045749	-0.84078832	3093.4129, 3098.3005, 3122.4747,
	C	-2.94990732	-1.03474125	0.20459787	3123.1739, 3130.4983, 3131.7262
	H	-3.72174795	-0.34397564	0.54774993	
	H	-2.57494146	-1.56967276	1.07857335	
	H	-3.42051998	-1.76172475	-0.45645843	
n-heptane_15	C	2.77592844	0.77037155	-0.01483612	61.7254, 82.8585, 140.3683, 196.5500,
	H	2.41153054	1.57476400	-0.65651477	224.5368, 239.7364, 271.5629,
	H	3.34536641	1.22215560	0.79662303	303.0585, 365.0541, 419.9716,
	H	3.45982938	0.16124398	-0.60776792	503.5075, 732.7903, 749.9134,
	C	0.82937264	-0.72659657	-0.62065412	791.4233, 833.3047, 866.8877,
	H	0.49025837	0.03752923	-1.32615856	902.3895, 953.6710, 963.5622,
	H	1.50724796	-1.37176395	-1.18621823	1043.2466, 1059.9605, 1065.0157,
	C	1.61571306	-0.06739959	0.50659882	1080.4004, 1128.8585, 76.7962,
	H	1.98895150	-0.84368897	1.18014101	1237.6938, 1252.6358, 1304.9683,
	H	0.95431245	0.56309402	1.10420926	1305.9327, 1327.3832, 1339.9346,
	C	-0.36056692	-1.55738312	-0.14744034	1369.3779, 1387.9600, 1395.6362,
	H	0.00335667	-2.35064676	0.51162383	1406.6353, 1412.4468, 1414.5200,
	H	-0.80604881	-2.05650559	-1.01209386	1486.5348, 1488.2590, 1490.9577,
	C	-1.46437406	-0.78264111	0.57665879	1498.1818, 1501.9081, 1503.4223,
	H	-1.08434844	-0.37555577	1.51741711	1507.1467, 1510.2108, 1518.8953,
	H	-2.23822897	-1.50047124	0.85411918	3038.4765, 3042.4363, 3046.7319,
	C	-2.09857376	0.34813726	-0.24502366	3050.7876, 3052.7492, 060.8329,
	H	-2.07276254	0.07976902	-1.30516007	3069.5937, 3078.1188, 3087.5280,
	H	-3.15414024	0.43118055	0.01884281	3092.0870, 3094.9554, 3119.5570,
	C	-1.45287579	1.71722773	-0.04389754	

	H	-0.40864940	1.73123591	-0.35340482	3123.1040, 3130.9137, 3142.2765
	H	-1.48711137	2.00254871	1.00892670	
	H	-1.97730520	2.48481433	-0.61301968	
n-heptane_16	C	3.15267538	0.84214480	0.00033217	
	H	3.08456036	1.27292337	1.00034891	79.0140, 85.2244, 109.3674, 157.7777,
	H	4.19579508	0.58737076	-0.18398178	183.7635, 218.8560, 249.7863,
	H	2.86585999	1.61658271	-0.71252564	302.9165, 371.6344, 402.3542,
	C	0.77935864	-0.04182501	0.12886434	475.5259, 738.0350, 757.1710,
	H	0.67312443	0.37619934	1.13561813	788.6304, 833.9017, 870.5440,
	H	0.46890388	0.74404734	-0.56571338	925.8633, 952.4228, 980.3887,
	C	2.24438495	-0.37370358	-0.12740984	1043.2700, 1049.5760, 1073.0219,
	H	2.34318935	-0.80533916	-1.12694799	1091.4487, 1122.4065, 11.4009,
	H	2.56381965	-1.14896808	0.57374784	1240.2901, 1263.2407, 1292.0734,
	C	-0.13316744	-1.25320392	-0.01981512	1311.1592, 1327.5027, 1333.6042,
	H	0.25112815	-2.06202805	0.60790443	1366.5797, 1379.1209, 1388.9308,
	H	-0.07316606	-1.61286358	-1.05195240	1409.7115, 1412.8725, 1413.8478,
	C	-1.59948862	-1.00614455	0.33232767	1483.8791, 1489.1678, 1493.5097,
	H	-1.67768274	-0.74881830	1.39319027	1498.7381, 1502.1266, 1502.9493,
	H	-2.13889375	-1.94644707	0.20709104	1504.8846, 1511.3895, 1514.2960,
	C	-2.27829714	0.09030734	-0.50133484	3028.0645, 3036.3858, 3039.9862,
	H	-1.79261075	0.15031319	-1.47948416	3048.1562, 3049.0659, 39.9491,
	H	-3.31439507	-0.19017603	-0.69660438	3062.2315, 3073.5189, 3083.8821,
	C	-2.27049428	1.46320041	0.16547591	3091.7413, 3094.2116, 3122.7405,
	H	-1.25872487	1.79596701	0.39333010	3125.3511, 3131.5730, 3141.2729
	H	-2.82381356	1.43042666	1.10510019	
	H	-2.73692295	2.21615690	-0.46976287	
n-heptane_17	C	2.92333201	-0.67914245	0.28210137	
	H	2.86809686	-0.65380493	1.37149725	61.4477, 100.0299, 108.9866,
	H	3.31599269	-1.65235305	-0.01051065	186.8973, 214.7815, 247.0968,
	H	3.64202839	0.08060573	-0.02892593	269.9209, 299.5119, 369.0351,
	C	1.00575097	0.95656726	0.05149577	418.4861, 499.9921, 727.7814,
	H	0.94390143	1.02574829	1.14291604	749.5457, 788.2692, 857.4576,
	H	1.74056563	1.70535494	-0.25456946	873.8932, 881.9485, 951.2867,
	C	1.55583206	-0.41474299	-0.33423989	965.6985, 1030.0310, 1060.8259,
	H	1.62517360	-0.47120332	-1.42398389	1073.4278, 1080.1749,
	H	0.86176099	-1.20027870	-0.03201841	1124.2672, 180.2597, 1232.6356,
	C	-0.35930921	1.30085706	-0.55890478	1263.5343, 1283.8255, 1317.0022,
	H	-0.46305705	0.79412709	-1.52225937	1331.4684, 1336.6860, 1365.3820,
	H	-0.39540210	2.36890604	-0.77956308	1390.4993, 1395.3106, 1400.2511,
	C	-1.55637549	0.97628684	0.33712830	1411.1030, 1415.7343, 1483.3640,
	H	-2.47086917	1.30770872	-0.16299549	1485.3454, 1495.7584, 1497.8901,
	H	-1.47105483	1.57147089	1.25021222	1498.6228, 1502.8270, 1507.2365,
	C	-1.71644222	-0.49364280	0.71950472	1512.3813, 1519.3696, 3031.2630,
	H	-0.83292835	-0.82992428	1.26735355	3039.4216, 3049.8199, 3052.4711,
	H	-2.55195607	-0.58130119	1.41688666	3056.04493059.7759, 3070.4831,
	C	-1.96899824	-1.40472879	-0.47617831	3078.5778, 3088.6999, 3093.8483,
	H	-1.13029428	-1.39888609	-1.17240132	3101.2966, 3123.6437, 3125.7269,
	H	-2.85449155	-1.07934111	-1.02514315	3131.4718, 3134.5292
	H	-2.13020549	-2.43555383	-0.16193802	
n-heptane_18	C	-2.56561943	0.26199431	-0.72116511	
	H	-3.28814228	-0.31907709	-0.14479778	71.9836, 103.7450, 118.1654,
	H	-3.11108270	1.03552090	-1.26052715	199.7149, 214.5738, 254.2087,
	H	-2.12111391	-0.40421257	-1.46104610	290.8929, 359.8657, 370.0316,
	C	-0.82115327	-0.16306229	1.08805431	442.2801, 504.4240, 726.5168,
	H	-0.08438704	0.33465138	1.72242899	746.1389, 794.2826, 830.4629,
	H	-1.56843952	-0.58302787	1.76714040	865.8745, 899.2061, 955.9649,
	C	-1.50524431	0.86844647	0.19139345	960.3623, 1017.1697, 1054.8431,
	H	-0.76067673	1.38706426	-0.41605687	1063.2809, 1089.9015,

	H	-1.96447267	1.63039572	0.82424653	1129.0309,168.7715, 1232.7266,
	C	-0.15526695	-1.31547913	0.33634852	1247.2109, 1294.9929, 1310.6171,
	H	-0.92459640	-1.90173892	-0.17141294	1331.9467, 1364.8156, 1373.4298,
	H	0.30225469	-1.98857096	1.06624220	1382.3459, 1398.6574, 1402.4619,
	C	0.91122165	-0.91664347	-0.68495934	1414.1914, 1416.0025, 1483.1395,
	H	0.47054455	-0.28233687	-1.46023279	1486.6809, 1490.9583, 1499.5717,
	H	1.23248999	-1.82811353	-1.19230109	1500.9301, 1508.5383, 1511.1910,
	C	2.14486764	-0.21832968	-0.09675256	1512.4210, 1518.1796, 3042.0895,
	H	2.34480450	-0.62549583	0.89864654	3044.2741, 3047.0401, 3051.4035,
	H	3.01470667	-0.47100774	-0.70553235	3056.05383061.5357, 3076.4267,
	C	2.05148377	1.30354315	-0.02031711	3083.5220, 3089.3260, 3092.1509,
	H	1.26358603	1.63687954	0.65266152	3096.4551, 3122.4491, 3123.4205,
	H	1.84315934	1.72310081	-1.00613685	3131.1175, 3147.7571
	H	2.98963088	1.73315255	0.33106477	
n-heptane_19	C	-3.10539448	-0.26223023	-0.32801618	
	H	-3.34875923	-0.85449373	0.55625186	48.0645, 89.6559, 137.2616, 145.9797,
	H	-4.03014277	0.17516451	-0.70270502	230.4119, 263.9136, 304.4203,
	H	-2.73052998	-0.94399682	-1.09096344	319.8097, 327.3623, 431.0646,
	C	-0.81520974	0.26817521	0.66379219	499.4224, 731.5702, 768.6361,
	H	-0.15438596	1.09889411	0.91744587	794.4029, 830.5752, 876.2888,
	H	-1.07579630	-0.21378202	1.61150637	909.8092, 948.3791, 961.8159,
	C	-2.08123008	0.81563771	0.01057957	1015.8148, 1065.2050, 1071.3247,
	H	-1.80643059	1.35540991	-0.90014225	1097.2396, 1119.3662,183.9961,
	H	-2.53723054	1.54956356	0.67777220	1236.9596, 1255.1911, 1296.0564,
	C	-0.06029065	-0.73908204	-0.20291548	1313.5221, 1324.3919, 1342.2923,
	H	0.03871891	-0.33964646	-1.21877652	1378.1266, 1380.4599, 1383.5064,
	H	-0.66238685	-1.64412587	-0.29358419	1400.4160, 1414.3171, 1415.6478,
	C	1.32985706	-1.09804617	0.34102558	1484.7697, 1489.4009, 1492.4578,
	H	1.52601518	-2.15978744	0.18416512	1494.2153, 1503.7066, 1504.8714,
	H	1.34151976	-0.94187846	1.42436233	1509.2529, 1512.1046, 1516.7503,
	C	2.47115673	-0.30453514	-0.29524275	3027.1998, 3038.2345, 3042.8055,
H	3.41769765	-0.63904764	0.13418773	3047.9874, 3048.17343057.5978,	
H	2.51360325	-0.54793799	-1.36026070	3079.8998, 3084.4165, 3087.1394,	
C	2.35175054	1.20629066	-0.13339524	3092.1435, 3106.0671, 3122.8457,	
H	2.29181016	1.48316322	0.92068347	3124.2474, 3128.5507, 3134.8384	
H	1.45942695	1.59017885	-0.62951607		
H	3.21303416	1.71506230	-0.56539300		
n-heptane_20	C	-1.64861486	1.53573628	-0.25858636	
	H	-2.26156186	1.47865692	-1.16002731	59.7882, 106.9134, 148.6576,
	H	-1.94342260	2.42941573	0.29068873	190.5732, 224.4284, 263.6651,
	H	-0.61317051	1.66878767	-0.57375968	281.7646, 314.7551, 392.9230,
	C	-1.50922583	-1.00859106	-0.16749486	423.1864, 484.6736, 737.0606,
	H	-1.70438722	-1.86012877	0.48992008	756.8050, 789.5519, 836.1299,
	H	-2.20750249	-1.09870714	-1.00453840	874.7021, 878.6991, 944.5837,
	C	-1.82331059	0.28079074	0.58885366	963.9747, 1004.9242, 1055.4025,
	H	-1.20143195	0.34442721	1.48449679	1073.6461, 1084.0541, 1134.0899,
	H	-2.85465694	0.23047124	0.94379354	69.5404, 1220.4690, 1263.9836,
	C	-0.08252688	-1.13274135	-0.70663220	1284.2443, 1315.6103, 1329.8186,
	H	0.10349370	-0.35260105	-1.44778146	1356.4916, 1375.4649, 1390.0306,
	H	-0.02121237	-2.07534433	-1.25313323	1393.5726, 1399.6202, 1412.2900,
	C	1.01177367	-1.11215413	0.36966621	1416.2581, 1482.9138, 1486.6009,
	H	1.84093612	-1.74719847	0.04708070	1488.6857, 1496.5272, 1501.0960,
	H	0.61581460	-1.57114405	1.28027897	1503.9495, 1508.8741, 1513.2446,
	C	1.59515926	0.26242956	0.70928794	1519.2588, 3038.1048, 3038.8071,
H	0.80776510	0.94362050	1.03372959	3054.7714, 3057.0711,	
H	2.26817660	0.14818760	1.56164573	3059.5483,067.2535, 3074.2405,	
C	2.36715093	0.89166491	-0.44528249	3079.6626, 3090.3743, 3098.6247,	
H	1.72325355	1.09333691	-1.30174172	3105.8915, 3123.8629, 3128.1999,	

	H	3.16569537	0.22853855	-0.78242056	3131.4017, 3132.8904
	H	2.81977667	1.83687182	-0.14710326	
n-heptane_21	C	-2.91505683	0.05894907	0.76898009	59.1247, 90.1143, 128.2289, 149.1372, 220.6330, 223.1210, 264.0476, 303.8874, 376.2122, 411.5692, 508.7986, 741.6304, 772.4701, 788.8177, 825.1908, 866.5860, 914.3820, 954.4301, 972.5420, 1025.2638, 1050.7330, 1073.6209, 1094.6903, 1121.9241, 183.4289, 1233.1134, 1263.1998, 1296.6923, 1310.1238, 1329.7552, 1347.4719, 1368.8691, 1377.2544, 1387.5717, 1408.2382, 1413.1420, 1416.1463, 1482.2784, 1491.5856, 1493.6420, 1498.0554, 1502.0475, 1504.2032, 1508.6790, 1512.0768, 1513.2436, 3033.3383, 3038.7461, 3042.4128, 3047.1581, 3047.96773062.3600, 3067.7790, 3080.8177, 3085.1076, 3091.7523, 3095.6854, 3124.8082, 3124.9767, 3136.5039, 3144.0685
	H	-2.53852888	0.64555559	1.60926261	
	H	-3.99365962	0.20312970	0.71689116	
	H	-2.73360079	-0.99234030	0.99054794	
	C	-0.71282046	0.43032381	-0.46474463	
	H	-0.29943973	0.80302009	-1.40633496	
	H	-0.36924410	1.11320495	0.31794523	
	C	-2.23777726	0.48254678	-0.52990387	
	H	-2.58279016	-0.15742733	-1.34643342	
	H	-2.54757631	1.49846378	-0.78218918	
	C	-0.16327118	-0.96808130	-0.20045972	
	H	-0.63950064	-1.66857051	-0.89342737	
	H	-0.45017675	-1.28743613	0.80491463	
	C	1.35436189	-1.09209001	-0.33140074	
	H	1.64924346	-0.86371691	-1.36035922	
	H	1.62271677	-2.13617075	-0.16182199	
	C	2.15059157	-0.19782115	0.63012770	
H	1.56109207	-0.03197461	1.53643394		
H	3.05247640	-0.72231483	0.94938592		
C	2.56421251	1.14310126	0.02966492		
H	1.70335900	1.71964040	-0.30565321		
H	3.21157923	0.98738925	-0.83452868		
H	3.11260868	1.74797688	0.75178410		
n-heptane_22	C	1.71267989	-1.41767191	0.39573390	56.7841, 87.0850, 129.1305, 200.9512, 217.7685, 266.8160, 269.2875, 356.8340, 368.1777, 414.7378, 481.2567, 728.2697, 758.0232, 792.0923, 819.9548, 838.2553, 908.7930, 950.9689, 965.1656, 1034.0274, 1061.8310, 1063.5374, 1096.5417, 1137.4634, 178.8738, 1235.9703, 1236.6227, 1306.4313, 1319.1182, 1329.5719, 1364.7285, 1378.5455, 1385.4942, 1394.2637, 1403.8675, 1413.3922, 1415.3126, 1484.2523, 1484.5032, 1490.0112, 1496.7773, 1498.4849, 1503.5648, 1506.6127, 1515.1539, 1520.2390, 3035.0795, 3045.7949, 3045.9820, 3051.3925, 3056.22873063.8787, 3071.0364, 3085.7763, 3086.2061, 3091.9664, 3092.0695, 3123.1814, 3123.4369, 3153.6297, 3154.8570
	H	1.54801812	-2.00489288	-0.50919364	
	H	2.51576468	-1.89388545	0.95836820	
	H	0.80584613	-1.47954598	0.99388594	
	C	1.04189995	0.77769055	-0.80020730	
	H	1.57133871	1.50072935	-1.42391900	
	H	0.55368472	0.09027803	-1.49537785	
	C	2.07767288	0.02114704	0.04332076	
	H	2.26762036	0.58678198	0.95987180	
	H	3.02464831	0.00304998	-0.49914901	
	C	0.00000608	1.56297660	0.00000146	
	H	-0.53969297	2.22147541	-0.68659002	
	H	0.53970849	2.22146919	0.68659622	
	C	-1.04189104	0.77769155	0.80020730	
	H	-1.57132415	1.50073049	1.42392363	
	H	-0.55367893	0.09027224	1.49537355	
	C	-2.07767121	0.02115922	-0.04332204	
H	-3.02464695	0.00307205	0.49914747		
H	-2.26761257	0.58679658	-0.95987289		
C	-1.71269454	-1.41766412	-0.39573453		
H	-1.54803923	-2.00488644	0.50919332		
H	-0.80586185	-1.47954926	-0.99388679		
H	-2.51578498	-1.89386890	-0.95836820		
SP1_1	C	3.23890267	-0.68534176	0.34260416	692.6573i, 42.9901, 48.2636, 74.9928, 98.6893, 106.6981, 110.2320, 148.7313, 165.0273, 246.8542, 248.3562, 308.9079, 321.6261, 422.0942, 489.0034, 723.0002, 729.0589, 763.7419, 801.0695, 848.4981, 892.1520, 918.9155, 942.8630, 1018.2534, 1026.2624, 1063.3114, 1082.1384, 1090.1996,
	H	4.07849045	-1.27645412	-0.01910354	
	H	3.46371150	0.39122311	-0.03475839	
	H	3.25700789	-0.63766277	1.43136590	
	C	0.75084052	-0.23528868	0.27313834	
	H	0.72974664	-0.23422952	1.36792018	
	H	0.94491258	0.79535242	-0.03781423	
	C	1.89734200	-1.11628483	-0.20647071	
	H	1.92816386	-1.11052266	-1.29830229	
H	1.70635081	-2.15286430	0.09150997		

	C	-0.60643178	-0.67789209	-0.25680023	1097.0727, 1154.6258, 1188.9397,
	H	-0.79701261	-1.71111039	0.05006641	1218.8813, 1243.3380, 1262.3618,
	H	-0.58167066	-0.68291648	-1.35080424	1284.8658, 1312.7509, 1326.8170,
	C	-1.75186515	0.20719631	0.21615681	1332.9397, 1339.4754, 1360.8694,
	H	-1.56214129	1.24005086	-0.09231451	1375.4538, 1404.6649, 1410.4806,
	H	-1.77633257	0.21478655	1.31057167	1414.7878, 1457.6082, 1479.8576,
	C	-3.11080764	-0.23331258	-0.31291899	1486.5462, 1488.8115, 1497.6648,
	H	-3.08419020	-0.24026488	-1.40558302	1503.1966, 1507.5081, 1514.6819,
	H	-3.29798698	-1.26506634	-0.00426065	1517.6546, 3029.6154, 3029.9062,
	C	-4.24512613	0.66179779	0.16841375	3033.5613, 3040.3118, 3049.6395,
	H	-4.08833694	1.69227273	-0.15354254	3054.6736, 3057.2941, 3064.5334,
	H	-4.30291448	0.66177637	1.25785690	3075.4626, 3084.1945, 3090.0615,
	H	-5.20931772	0.33332944	-0.21797793	3096.9700, 3123.6630, 3131.3341,
	O	3.54101053	1.79253168	-0.34424252	3152.5087, 3785.5297
	H	3.22630841	2.11680153	0.51437167	
	C	-3.20384834	-0.71124279	0.39244880	
	H	-3.19656215	-0.86345989	1.47191921	706.0480i, 39.6019, 42.6791, 73.9573,
	H	-3.37912406	0.42986840	0.26632779	96.1177, 107.4551, 113.0274,
	H	-4.06220349	-1.21272664	-0.05078431	147.9285, 157.9762, 247.3000,
	C	-0.71661429	-0.27826176	0.33270885	250.1244, 307.8366, 326.4572,
	H	-0.92007479	0.79269313	0.24692339	423.1538, 488.2515, 720.5743,
	H	-0.65175995	-0.49712323	1.40314842	728.9149, 764.7862, 783.7547,
	C	-1.88543853	-1.04969967	-0.26690825	838.3713, 898.4899, 925.7202,
	H	-1.70079379	-2.12514652	-0.17260589	930.9329, 1016.4198, 1025.1617,
	H	-1.94721585	-0.84024941	-1.33757730	1064.1791, 1087.7238, 1089.0295,
	C	0.61491724	-0.60153224	-0.33130299	1100.7371, 1157.3533, 1174.0492,
	H	0.54782582	-0.37967764	-1.40093355	1224.0208, 1257.4690, 1280.0958,
	H	0.80983247	-1.67592413	-0.25308295	1295.9302, 1315.6604, 1327.7916,
	C	1.78487085	0.16697520	0.26850350	1331.7801, 1342.1260, 1363.3527,
	H	1.85401246	-0.05498512	1.33814175	1371.7642, 1404.4723, 1410.5707,
	H	1.58905821	1.24096442	0.19199617	1415.2530, 1453.6865, 1479.7540,
	C	3.11793052	-0.15002516	-0.39713523	1486.0256, 1488.6765, 1497.1449,
	H	3.31047850	-1.22335217	-0.32067909	1503.8117, 1506.6705, 1514.2788,
	H	3.04690077	0.07335168	-1.46477777	1523.4368, 3029.8068, 3032.3729,
	C	4.27728379	0.62550135	0.21458219	3035.0034, 3042.7442, 3049.6570,
	H	4.37948716	0.39565199	1.27614677	3055.1178, 3057.9626, 3066.2835,
	H	4.11425677	1.70037889	0.12432006	3073.2748, 3085.0382, 3089.4797,
	H	5.22265202	0.38797595	-0.27205388	3097.5942, 3124.1638, 3132.0359,
	O	-3.57829009	1.78175299	-0.19286998	3151.9915, 3787.3677
	H	-4.32505691	1.58744681	-0.78085026	
SP1_2	C	-2.51791135	0.78438528	0.08710137	
	H	-3.15365126	1.41262509	0.70777406	770.0318i, 50.1400, 58.3739, 74.1082,
	H	-1.60414835	1.47609965	-0.13836937	120.3300, 151.0925, 164.9278,
	H	-2.98068158	0.62501468	-0.88751717	191.5149, 240.0874, 257.2931,
	C	-1.40951190	-1.50095434	-0.15792650	289.9062, 353.0095, 395.0874,
	H	-1.18800225	-2.41243281	0.40312782	404.7706, 495.0152, 669.5322,
	H	-2.10637156	-1.78554450	-0.95030735	735.5766, 762.1186, 824.9352,
	C	-2.11088435	-0.50631984	0.76712460	853.7401, 876.8979, 921.2026,
	H	-1.48934944	-0.28568970	1.63745813	950.0008, 974.5175, 1020.3427,
	H	-3.01306382	-0.98141650	1.16309452	1048.4867, 1067.9870, 1087.4219,
	C	-0.12275287	-0.98049828	-0.79451132	1096.2967, 1124.2716, 1159.9944,
	H	-0.34073997	-0.09188079	-1.39394216	1173.9803, 1237.4218, 1247.0824,
	H	0.25523224	-1.72944228	-1.49459837	1284.5117, 1298.1043, 1325.3210,
	C	0.97736431	-0.66091139	0.21208414	1328.6413, 1334.0074, 1371.4899,
	H	1.23019867	-1.56674917	0.77209404	1388.8646, 1395.6049, 1411.0651,
	H	0.61541754	0.04893101	0.96477768	1416.6175, 1443.0595, 1485.5048,
	C	2.23770497	-0.10312752	-0.44016631	1492.6357, 1495.3736, 1500.0732,
	H	2.61839607	-0.83386534	-1.15779853	1503.7545, 1506.7563, 1517.3929,
SP1_3	C	-2.51791135	0.78438528	0.08710137	
	H	-3.15365126	1.41262509	0.70777406	770.0318i, 50.1400, 58.3739, 74.1082,
	H	-1.60414835	1.47609965	-0.13836937	120.3300, 151.0925, 164.9278,
	H	-2.98068158	0.62501468	-0.88751717	191.5149, 240.0874, 257.2931,
	C	-1.40951190	-1.50095434	-0.15792650	289.9062, 353.0095, 395.0874,
	H	-1.18800225	-2.41243281	0.40312782	404.7706, 495.0152, 669.5322,
	H	-2.10637156	-1.78554450	-0.95030735	735.5766, 762.1186, 824.9352,
	C	-2.11088435	-0.50631984	0.76712460	853.7401, 876.8979, 921.2026,
	H	-1.48934944	-0.28568970	1.63745813	950.0008, 974.5175, 1020.3427,
	H	-3.01306382	-0.98141650	1.16309452	1048.4867, 1067.9870, 1087.4219,
	C	-0.12275287	-0.98049828	-0.79451132	1096.2967, 1124.2716, 1159.9944,
	H	-0.34073997	-0.09188079	-1.39394216	1173.9803, 1237.4218, 1247.0824,
	H	0.25523224	-1.72944228	-1.49459837	1284.5117, 1298.1043, 1325.3210,
	C	0.97736431	-0.66091139	0.21208414	1328.6413, 1334.0074, 1371.4899,
	H	1.23019867	-1.56674917	0.77209404	1388.8646, 1395.6049, 1411.0651,
	H	0.61541754	0.04893101	0.96477768	1416.6175, 1443.0595, 1485.5048,
	C	2.23770497	-0.10312752	-0.44016631	1492.6357, 1495.3736, 1500.0732,
	H	2.61839607	-0.83386534	-1.15779853	1503.7545, 1506.7563, 1517.3929,

	H	1.98215372	0.78460244	-1.02767339	1522.5865, 3024.9895, 3037.6401,
	C	3.32049612	0.24287963	0.57321305	3042.7552, 3050.0806, 3050.7430,
	H	3.60710231	-0.63799887	1.14918091	3055.6706, 3057.1563, 3074.9051,
	H	2.96644317	0.99694348	1.27808895	3076.8371, 3083.4388, 3093.3353,
	H	4.21455654	0.63276141	0.08859802	3096.1078, 3121.8748, 3134.8096,
	O	-0.50620309	2.36974969	-0.31540464	3154.4708, 3782.9601
	H	0.18910301	1.73732351	-0.07226487	
SP1_4	C	2.89725545	-0.07103846	0.59516692	771.1119i, 57.9339, 64.2050, 70.9459,
	H	3.97995103	-0.00224854	0.50952189	112.5468, 118.5233, 137.7737,
	H	2.55009915	1.01328426	0.34557209	171.2417, 208.3117, 245.6579,
	H	2.61011300	-0.23449843	1.63449599	272.0147, 328.4953, 360.0510,
	C	0.82721679	-1.40915983	-0.06788303	398.2492, 498.1551, 672.0463,
	H	0.48862483	-2.17672322	-0.76813910	738.7472, 774.0417, 828.1741,
	H	0.75165627	-1.84814306	0.93159746	846.8033, 889.4405, 922.7040,
	C	2.28857509	-1.07859920	-0.35900543	948.0053, 992.4767, 1029.1443,
	H	2.38800657	-0.71259479	-1.38454784	1053.1437, 1078.3867, 1093.3978,
	H	2.87360108	-2.00101816	-0.30895939	1111.8025, 1138.1922, 1175.9860,
	C	-0.11434275	-0.21372702	-0.15306535	1220.7553, 1247.5490, 1256.3156,
	H	0.00864234	0.27142484	-1.12951840	1289.4768, 1304.5505, 1324.4060,
	H	0.15575728	0.52314997	0.60958548	1331.4157, 1337.7408, 1346.9388,
	C	-1.57809545	-0.59377037	0.02953993	1389.3539, 1397.2886, 1408.2176,
	H	-1.70120644	-1.09593669	0.99417412	1414.8937, 1437.2053, 1480.5773,
	H	-1.86059905	-1.32504408	-0.73401190	1488.2066, 1493.3508, 1496.2407,
	C	-2.52240038	0.59952542	-0.04094768	1503.4783, 1508.7742, 1510.4383,
	H	-2.23771530	1.32757332	0.72299457	1521.0785, 3010.1043, 3033.7886,
H	-2.39587132	1.09999098	-1.00467352	3041.1345, 3044.1769, 3048.0516,	
C	-3.98120073	0.20316453	0.14399822	3055.4966, 3057.8569, 3066.7155,	
H	-4.13249924	-0.27500438	1.11273453	3073.6325, 3083.8309, 3088.6821,	
H	-4.29083368	-0.50509769	-0.62576583	3094.1787, 3124.1672, 3132.9847,	
H	-4.64256711	1.06700976	0.09006263	3155.1826, 3787.5805	
O	2.15589962	2.28389003	-0.16924010		
H	1.30559559	1.98438525	-0.52802334		
SP1_5	C	2.57150245	0.40358604	-0.21458700	650.3585i, 24.6746, 36.0680, 61.0650,
	H	2.79410155	0.23302924	-1.26843667	82.9574, 116.4827, 136.3579,
	H	1.70588436	1.17807832	-0.21407267	205.0934, 230.4193, 257.2453,
	H	3.41257279	0.89441118	0.27172831	296.0042, 347.6821, 363.6164,
	C	1.02344070	-1.61507824	-0.24269996	434.9081, 507.8703, 678.3573,
	H	1.44207859	-1.98507086	-1.18257059	737.6979, 763.3528, 821.5152,
	H	0.74930094	-2.49657732	0.34256106	852.0614, 857.1013, 905.4832,
	C	2.11306762	-0.84829620	0.50530613	954.8289, 966.6980, 1013.5784,
	H	2.97847800	-1.50450947	0.63801687	1048.9591, 1072.2268, 1093.5117,
	H	1.77601929	-0.58890770	1.51025476	1120.1652, 1136.9470, 1156.8069,
	C	-0.23624182	-0.80364297	-0.54529523	1180.8581, 1231.2846, 1243.2650,
	H	-0.92184000	-1.44005916	-1.10789422	1292.7277, 1298.8732, 1334.2252,
	H	0.00808629	0.03895062	-1.19862327	1337.8462, 1348.4951, 1376.6106,
	C	-0.93660358	-0.27143717	0.70037668	1379.6931, 1391.4448, 1408.5769,
	H	-0.23783922	0.33787785	1.27579394	1416.3530, 1451.0513, 1480.5539,
	H	-1.22603423	-1.11449182	1.33783418	1486.3928, 1492.1705, 1494.3339,
	C	-2.16505561	0.58046165	0.39004443	1503.8142, 1505.5747, 1513.0427,
	H	-2.56091615	0.98054679	1.32554352	1580.0618, 3026.6734, 3039.3017,
H	-1.84908827	1.44073986	-0.20484901	3047.7040, 3053.1487, 3055.5979,	
C	-3.27110748	-0.17561422	-0.33831883	3057.1239, 3076.6959, 3081.8601,	
H	-3.55129411	-1.07711656	0.21050302	3086.4698, 3089.9103, 3099.3518,	
H	-2.96049459	-0.47882091	-1.33779130	3107.5623, 3122.5975, 3134.3702,	
H	-4.16364046	0.44012970	-0.44614947	3150.5777, 3787.5202	
O	0.81414902	2.31495945	-0.16963135		
H	1.49741940	3.00224128	-0.12375507		
SP1_6	C	-3.10421686	-0.85186340	-0.05613589	691.8743i, 27.7179, 56.2268, 83.2049,

	H	-3.83133478	-1.44724396	0.49339101	94.1633, 112.6064, 127.5070,
	H	-3.37697580	0.24709307	0.20850858	147.6817, 162.5330, 246.2239,
	H	-3.26878404	-0.95752020	-1.12838997	289.8154, 321.2950, 357.7682,
	C	-0.68063156	-0.21339460	-0.39738231	398.8201, 497.7240, 723.9829,
	H	-0.80725628	-0.35699824	-1.47547890	742.0402, 773.9320, 800.2796,
	H	-0.92260792	0.83316689	-0.18988874	847.3347, 881.4017, 910.5502,
	C	-1.66849284	-1.10204323	0.34761353	949.4655, 985.5663, 1027.1986,
	H	-1.55705140	-0.94795021	1.42318864	1055.1804, 1076.3793, 1095.6457,
	H	-1.42312000	-2.15279170	0.15906057	1107.6197, 1150.1225, 1181.9692,
	C	0.77018917	-0.48161742	-0.01920732	1212.8399, 1241.3768, 1266.2768,
	H	1.01690604	-1.52605765	-0.23788923	1284.7324, 1314.6236, 1324.2187,
	H	0.88148300	-0.35799326	1.06091089	1335.5567, 1352.0788, 1365.3641,
	C	1.74862685	0.43027211	-0.75079758	1379.1862, 1398.4268, 1411.1722,
	H	1.55210623	1.46799377	-0.46332623	1415.7063, 1457.6075, 1479.6517,
	H	1.55393806	0.36600014	-1.82476000	1484.3199, 1492.7283, 1494.5029,
	C	3.21694302	0.10498908	-0.48793928	1505.2828, 1510.5963, 1513.3623,
	H	3.42171840	-0.91658257	-0.81926221	1517.5639, 3029.6468, 3030.8272,
	H	3.83965569	0.75816757	-1.10211163	3035.0925, 3041.6261, 3047.8634,
	C	3.62057555	0.25627909	0.97463651	3058.7680, 3064.8315, 3070.8137,
	H	3.11010435	-0.46840451	1.60827703	3081.4612, 3085.8930, 3090.9998,
	H	3.37121932	1.25332316	1.34251097	3098.7906, 3125.6522, 3135.5566,
	H	4.69220668	0.10984402	1.10512790	3152.7692, 3788.3062
	O	-3.54009656	1.66825230	0.34438950	
	H	-3.34939504	1.89420537	-0.57971066	
	C	-3.03316805	-0.98113011	0.24596268	693.0276i, 26.6162, 53.8969, 86.0540,
	H	-3.08384931	-1.01381503	1.33425726	92.9658, 113.8735, 117.4361,
	H	-3.43822103	0.06225439	-0.06859308	150.5550, 162.2296, 240.9579,
	H	-3.74485443	-1.68489614	-0.18224114	287.0736, 318.8450, 357.4728,
	C	-0.66449723	-0.09570336	0.29531658	397.9624, 497.2160, 721.9690,
	H	-1.03676036	0.90456109	0.05587181	738.8938, 773.1423, 797.9053,
	H	-0.66258617	-0.17667907	1.38741145	844.4771, 886.1279, 910.1276,
	C	-1.62408556	-1.12761559	-0.28329918	946.5173, 983.8136, 1029.2797,
	H	-1.25825802	-2.13334501	-0.05009707	1053.0804, 1077.7869, 1095.0825,
	H	-1.63082644	-1.04730587	-1.37265002	1107.3383, 1147.1795, 1188.9244,
	C	0.75999680	-0.24517046	-0.22275294	1206.7529, 1242.6538, 1265.5912,
	H	0.75963589	-0.14885552	-1.31350169	1289.3093, 1305.1121, 1331.3942,
	H	1.11479530	-1.25528222	-0.00224980	1334.4467, 1350.3113, 1364.6795,
	C	1.71456426	0.78380267	0.37236846	1379.1762, 1398.4200, 1410.9900,
	H	1.77711143	0.62972802	1.45445991	1415.1378, 1456.0903, 1479.0891,
	H	1.29064270	1.78090760	0.22710473	1484.0394, 1491.9921, 1493.9231,
	C	3.11992722	0.74587846	-0.22272354	1504.5031, 1509.8071, 1511.7090,
	H	3.05904840	0.94814443	-1.29533034	1516.7377, 3029.4903, 3031.4653,
	H	3.70971729	1.55606976	0.21009510	3034.7986, 3043.9396, 3049.0653,
	C	3.84171928	-0.57779065	0.00523156	3058.2342, 3062.5017, 3071.0802,
	H	3.35019231	-1.39743551	-0.51810588	3081.0443, 3086.0770, 3090.6119,
	H	3.86406630	-0.82737904	1.06780008	3098.5303, 3125.3412, 3135.2376,
	H	4.87090030	-0.53191502	-0.34907351	3152.1566, 3788.4323
	O	-3.75959541	1.44559293	-0.29118818	
	H	-3.55073116	1.75687397	0.60372586	
SP1_7	C	-3.03316805	-0.98113011	0.24596268	693.0276i, 26.6162, 53.8969, 86.0540,
	H	-3.08384931	-1.01381503	1.33425726	92.9658, 113.8735, 117.4361,
	H	-3.43822103	0.06225439	-0.06859308	150.5550, 162.2296, 240.9579,
	H	-3.74485443	-1.68489614	-0.18224114	287.0736, 318.8450, 357.4728,
	C	-0.66449723	-0.09570336	0.29531658	397.9624, 497.2160, 721.9690,
	H	-1.03676036	0.90456109	0.05587181	738.8938, 773.1423, 797.9053,
	H	-0.66258617	-0.17667907	1.38741145	844.4771, 886.1279, 910.1276,
	C	-1.62408556	-1.12761559	-0.28329918	946.5173, 983.8136, 1029.2797,
	H	-1.25825802	-2.13334501	-0.05009707	1053.0804, 1077.7869, 1095.0825,
	H	-1.63082644	-1.04730587	-1.37265002	1107.3383, 1147.1795, 1188.9244,
	C	0.75999680	-0.24517046	-0.22275294	1206.7529, 1242.6538, 1265.5912,
	H	0.75963589	-0.14885552	-1.31350169	1289.3093, 1305.1121, 1331.3942,
	H	1.11479530	-1.25528222	-0.00224980	1334.4467, 1350.3113, 1364.6795,
	C	1.71456426	0.78380267	0.37236846	1379.1762, 1398.4200, 1410.9900,
	H	1.77711143	0.62972802	1.45445991	1415.1378, 1456.0903, 1479.0891,
	H	1.29064270	1.78090760	0.22710473	1484.0394, 1491.9921, 1493.9231,
	C	3.11992722	0.74587846	-0.22272354	1504.5031, 1509.8071, 1511.7090,
	H	3.05904840	0.94814443	-1.29533034	1516.7377, 3029.4903, 3031.4653,
	H	3.70971729	1.55606976	0.21009510	3034.7986, 3043.9396, 3049.0653,
	C	3.84171928	-0.57779065	0.00523156	3058.2342, 3062.5017, 3071.0802,
	H	3.35019231	-1.39743551	-0.51810588	3081.0443, 3086.0770, 3090.6119,
	H	3.86406630	-0.82737904	1.06780008	3098.5303, 3125.3412, 3135.2376,
	H	4.87090030	-0.53191502	-0.34907351	3152.1566, 3788.4323
	O	-3.75959541	1.44559293	-0.29118818	
	H	-3.55073116	1.75687397	0.60372586	
SP1_8	C	-2.90931912	-0.59277000	0.78408740	700.4257i, 26.1918, 59.3299, 75.2101,
	H	-3.32047457	-0.62874449	1.79149231	89.7131, 90.4086, 123.4536, 140.4074,
	H	-3.21740079	0.45713652	0.38896805	207.2241, 245.4593, 267.9884,
	H	-3.41590253	-1.31748420	0.14688850	313.4974, 323.4900, 407.2002,
	C	-0.85968904	-0.56983014	-0.69187132	518.0581, 724.3287, 738.2174,
	H	-1.40480249	-1.25822295	-1.34434391	779.8981, 793.8920, 850.9449,
	H	-1.07487746	0.44101543	-1.05060986	873.0983, 918.1251, 931.9268,
	C	-1.40231081	-0.70672815	0.72701051	989.6875, 1026.1519, 1058.0167,
	H	-0.95854414	0.05288039	1.37203109	

	H	-1.10091892	-1.67777920	1.13638639	1072.6898, 1093.7908, 1111.0923,
	C	0.63654237	-0.84450823	-0.81267234	1152.2525, 1174.1951, 1216.3830,
	H	0.92731821	-0.77612011	-1.86421321	1244.6663, 1268.1326, 1285.6591,
	H	0.84240031	-1.87425618	-0.50381810	1310.3753, 1319.2314, 1333.3065,
	C	1.50991648	0.10445460	0.00050157	1349.5535, 1364.1270, 1376.8372,
	H	1.31277620	-0.02751751	1.06772133	1404.4426, 1409.7750, 1413.7220,
	H	1.23893639	1.13876288	-0.23615231	1459.1733, 1479.2079, 1486.0031,
	C	2.99858956	-0.09853879	-0.25304250	1490.6283, 1500.6380, 1502.2573,
	H	3.26008720	-1.13736158	-0.03470254	1503.5772, 1513.7141, 1517.2357,
	H	3.20473661	0.05225690	-1.31579126	3025.7312, 3030.5327, 3037.4232,
	C	3.86756024	0.83651887	0.57761451	3039.1001, 3048.5306, 3057.0264,
	H	3.69725699	0.67910725	1.64359919	3061.6652, 3070.9270, 3077.5540,
	H	3.63459290	1.87919432	0.35702376	3085.4386, 3093.7949, 3102.9832,
	H	4.92791859	0.68143608	0.38147632	3123.2969, 3131.5156, 3153.1963,
	O	-3.50131460	1.66187838	-0.33912812	3789.4496
	H	-3.59032387	1.24908039	-1.21269777	
	C	2.97715858	-0.38283532	0.74263835	688.7859i, 29.6566, 63.6121, 77.9530,
	H	3.92742285	-0.91400247	0.73980681	98.4139, 105.8624, 121.7573,
	H	3.18436181	0.57767833	0.12133918	151.8701, 211.1571, 240.8962,
	H	2.73882268	-0.04888819	1.75241875	271.6066, 311.2297, 321.3426,
	C	0.54297538	-0.34713333	0.05389479	411.4335, 516.3177, 722.3224,
	H	0.28285405	-0.04929876	1.07341859	738.0871, 772.3533, 810.7317,
	H	0.70674068	0.57495423	-0.51263561	848.4226, 870.7678, 905.9450,
	C	1.84338179	-1.14047683	0.08892289	947.8958, 989.2550, 1031.7241,
	H	2.12663915	-1.42022396	-0.92818452	1056.7071, 1070.0901, 1091.3544,
	H	1.68035849	-2.07746806	0.63256542	1111.1986, 1153.0663, 1178.1752,
	C	-0.60705157	-1.12964948	-0.57012320	1215.9966, 1247.6150, 1273.4366,
	H	-0.82280220	-2.00603711	0.04928021	1287.2957, 1311.2612, 1324.6192,
	H	-0.28340895	-1.51202210	-1.54168112	1336.2612, 1345.5677, 1360.5191,
	C	-1.88458333	-0.31560622	-0.75422364	1383.5446, 1405.5089, 1410.3098,
	H	-2.63023894	-0.93041664	-1.26537531	1413.4691, 1456.8501, 1480.2686,
	H	-1.68071385	0.53229370	-1.41573788	1484.9310, 1490.6984, 1497.9352,
	C	-2.48783117	0.20266140	0.54705490	1503.0337, 1506.4854, 1512.5045,
	H	-2.61309713	-0.63316164	1.24148590	1519.2371, 3029.3651, 3033.6886,
	H	-1.79540580	0.89899526	1.02409215	3034.6970, 3043.7189, 3047.4760,
	C	-3.82644314	0.89523763	0.32574031	3056.4880, 3064.0283, 3068.6496,
	H	-4.55062310	0.20789287	-0.11370970	3076.9757, 3087.4980, 3092.1171,
	H	-3.71618658	1.73864133	-0.35754972	3098.0250, 3123.1096, 3131.5974,
	H	-4.24464993	1.27247465	1.25831744	3152.9199, 3786.4353
	O	3.20542167	1.84453857	-0.55847718	
	H	2.70091406	2.33909292	0.10654048	
SP1_9					
	C	-3.08613591	-0.34530937	0.39851506	688.2647i, 35.4672, 53.4715, 75.5807,
	H	-3.04534820	-0.28753924	1.48622417	82.7760, 101.3454, 117.8822,
	H	-3.04739719	0.74986444	0.01077673	150.4992, 208.9100, 243.6752,
	H	-4.06139691	-0.70964235	0.08033041	271.8004, 311.4832, 319.9722,
	C	-0.56944012	-0.53519624	0.22740929	411.2061, 515.8305, 720.1724,
	H	-0.52774375	0.51441824	-0.07220259	739.3082, 768.3235, 804.7693,
	H	-0.49423064	-0.55526160	1.32031431	857.9925, 869.6634, 905.7651,
	C	-1.91905429	-1.10204135	-0.19520553	944.4915, 989.8694, 1037.2427,
	H	-1.98315937	-2.15239247	0.10877388	1058.5440, 1064.8770, 1090.5242,
	H	-1.99157539	-1.09243906	-1.28519003	1111.6040, 1148.2881, 1191.5989,
	C	0.60447354	-1.30087927	-0.37226579	1210.2422, 1246.8024, 1267.4240,
	H	0.57046322	-1.20819945	-1.46220877	1299.4219, 1304.0238, 1324.9525,
	H	0.48267385	-2.36447992	-0.15015186	1333.5931, 1347.6464, 1357.5652,
	C	1.96920673	-0.83823122	0.12996091	1382.6471, 1405.5518, 1409.7365,
	H	2.74380579	-1.48380578	-0.29261965	1413.5852, 1456.6765, 1480.8590,
	H	2.01961132	-0.97018039	1.21564574	1484.7316, 1490.0960, 1497.8568,
	C	2.30136279	0.61056808	-0.21128150	
SP1_10					

	H	2.17345681	0.76287291	-1.28665179	1503.9832, 1506.7165, 1512.6229,
	H	1.59175376	1.27890506	0.28003768	1520.5078, 3028.4748, 3032.1007,
	C	3.71875720	0.98842807	0.19933314	3033.8890, 3040.4383, 3050.1569,
	H	4.45080010	0.36025651	-0.31016728	3056.3302, 3068.3206, 3069.7483,
	H	3.85918989	0.85330255	1.27292851	3077.2426, 3088.3024, 3093.2398,
	H	3.94403672	2.02723315	-0.03938437	3101.6689, 3123.0095, 3131.8425,
	O	-2.79033043	2.12736877	-0.31266659	3152.3046, 3788.7679
	H	-2.47731616	2.39410511	0.56608402	
SP1_11	C	2.94845209	0.76093858	-0.04765531	668.8976i, 29.1536, 35.5608, 62.1833,
	H	3.00599944	1.33079661	0.87949053	70.6690, 86.8324, 108.7161, 144.3454,
	H	3.92846217	0.14263000	-0.12363790	150.0288, 240.9733, 249.9860,
	H	2.97887292	1.43916740	-0.90013775	288.5365, 333.9755, 422.5732,
	C	0.43574043	0.54473257	-0.01062630	480.9459, 723.9234, 727.0577,
	H	0.39996982	1.14314626	0.90473586	742.7360, 779.3449, 848.6379,
	H	0.36631752	1.25154547	-0.84286627	906.9634, 932.6648, 962.9792,
	C	1.77291440	-0.19055447	-0.08236826	1018.2148, 1026.8634, 1063.1685,
	H	1.80904791	-0.78603592	-0.99701458	1070.2991, 1083.7333, 1091.8335,
	H	1.84420555	-0.89403580	0.75000810	1144.5660, 1206.1148, 1236.0205,
	C	-0.76029089	-0.39814667	-0.04607602	1247.2444, 1257.2148, 1291.2659,
	H	-0.68759271	-1.10540597	0.78575350	1307.5406, 1322.4917, 1331.7639,
	H	-0.72077557	-0.99689942	-0.96110056	1337.2072, 1344.2424, 1371.7716,
	C	-2.09714520	0.32793823	0.02446119	1396.2064, 1408.2888, 1413.9259,
	H	-2.16967299	1.03574825	-0.80729926	1456.1942, 1484.1681, 1485.8460,
	H	-2.13676346	0.92731791	0.93951471	1491.2926, 1499.6092, 1504.0527,
	C	-3.29460385	-0.61322557	-0.01125273	1508.7234, 1514.7241, 1518.9208,
	H	-3.25287587	-1.21085324	-0.92545040	3029.8246, 3032.8645, 3040.9266,
H	-3.22009212	-1.31911662	0.81993670	3049.5461, 3054.1387, 3057.0164,	
C	-4.62370645	0.12705197	0.05975360	3058.9749, 3063.0586, 3078.0153,	
H	-4.72716594	0.81850094	-0.77770288	3082.8805, 3090.2634, 3101.1221,	
H	-4.69382364	0.70992048	0.97927790	3123.1856, 3131.8163, 3147.0392,	
H	-5.46905475	-0.55961525	0.03342186	3792.7146	
H	5.12686292	-0.63283762	0.01201506		
H	5.44187516	-0.21651789	0.82953295		
SP1_12	C	-2.67076345	-0.38276320	0.86410303	681.4537i, 21.8345, 46.4736, 66.4602,
	H	-2.04050305	-0.29070874	1.74720541	83.6016, 103.2701, 115.7587,
	H	-2.75600443	0.70274205	0.46021923	137.1486, 185.3985, 247.6646,
	H	-3.67261558	-0.69043603	1.15768533	262.3054, 330.1249, 358.7460,
	C	-0.77705809	-0.67379135	-0.80864339	399.8050, 499.1217, 727.0134,
	H	-0.43004023	-1.33121859	-1.60976074	736.3461, 771.3688, 786.1540,
	H	-0.99260847	0.29516072	-1.26680206	848.2362, 881.2077, 917.7680,
	C	-2.07076329	-1.24186569	-0.22954498	946.0996, 984.8744, 1028.1525,
	H	-1.87983643	-2.24215702	0.17432982	1052.6376, 1083.5697, 1097.3011,
	H	-2.80037851	-1.36522952	-1.03150955	1106.4554, 1156.5875, 1166.3966,
	C	0.34070886	-0.50744180	0.21439513	1225.6925, 1256.1342, 1278.8308,
	H	0.48705689	-1.45028107	0.75276933	1286.4735, 1310.0856, 1334.0139,
	H	0.05246581	0.23562998	0.96261210	1335.0882, 1350.8848, 1365.0206,
	C	1.65787264	-0.07835825	-0.41911075	1383.9901, 1399.0141, 1411.0833,
	H	1.50431485	0.85302920	-0.97294110	1415.9504, 1451.2015, 1482.4666,
	H	1.96587898	-0.82563367	-1.15728816	1487.1041, 1488.5559, 1495.3423,
	C	2.77803467	0.11816339	0.59429778	1503.8358, 1505.1892, 1514.1457,
	H	2.47068060	0.86946948	1.32622291	1518.4648, 3027.1169, 3031.4530,
H	2.92450923	-0.81101527	1.15132865	3033.2011, 3047.1533, 3049.6534,	
C	4.08889023	0.54008741	-0.05639166	3056.2935, 3058.0507, 3071.1015,	
H	3.96746259	1.47982825	-0.59698707	3085.5856, 3088.4761, 3098.5959,	
H	4.42519216	-0.21113227	-0.77251157	3099.5264, 3122.5599, 3130.7217,	
H	4.87916284	0.67747067	0.68087284	3158.3184, 3789.1586	
O	-3.02452079	1.95040417	-0.21624983		
H	-3.99010028	1.85706534	-0.23007772		

SP1_13	C	2.71618140	1.19637970	0.17469358	702.8758i, 27.9236, 48.4513, 67.7727, 94.7209, 110.5822, 119.8094, 136.8566, 206.9442, 242.1058, 265.1912, 311.0751, 333.9813, 407.7167, 517.1658, 717.1334, 733.5585, 776.9929, 787.9207, 837.5569, 873.8037, 911.6685, 942.4729, 978.7876, 1033.2456, 1062.0924, 1068.6520, 1089.1170, 1109.7285, 1147.0713, 1182.0223, 1219.9765, 1256.4303, 1285.3380, 1295.5082, 1309.4800, 1330.6491, 1334.4632, 1343.5343, 1366.1717, 1377.0105, 1403.7698, 1409.6997, 1412.3763, 1454.8165, 1478.8928, 1485.2957, 1490.4060, 1498.2798, 1501.6159, 1502.5217, 1513.1054, 1526.7011, 3028.7239, 3035.7278, 3039.4746, 3043.8830, 3049.0971, 3057.0023, 3060.0887, 3071.0338, 3076.5064, 3085.9080, 3093.0122, 3096.6058, 3122.8522, 3132.0937, 3151.3524, 3786.7196
	H	2.77513566	1.47971834	1.22589067	
	H	3.41756686	0.27480135	0.09002233	
	H	3.14691457	1.97847036	-0.44786413	
	C	0.79061006	-0.37102224	0.61313408	
	H	1.53142821	-1.17364960	0.62297465	
	H	0.69447350	-0.02062392	1.64571108	
	C	1.32903241	0.76658589	-0.24836613	
	H	0.66010512	1.63033233	-0.19337585	
	H	1.34437763	0.45208059	-1.29554417	
	C	-0.55024203	-0.92308842	0.13904845	
	H	-0.82949693	-1.76960279	0.77165708	
	H	-0.43783815	-1.32211796	-0.87388547	
	C	-1.68529657	0.09467446	0.15181794	
	H	-1.47600250	0.89847877	-0.55941375	
	H	-1.73949179	0.56487336	1.13970349	
	C	-3.03719934	-0.52100524	-0.18729537	
	H	-2.97326940	-1.00725056	-1.16427515	
	H	-3.26143243	-1.31125581	0.53365963	
	C	-4.16383487	0.50372925	-0.19502894	
H	-3.97243363	1.28481264	-0.93225338		
H	-4.25563489	0.98552493	0.77951386		
H	-5.12325698	0.04609624	-0.43376722		
O	4.18850161	-0.87545169	-0.31308760		
H	4.59533579	-0.46459510	-1.09207456		
SP1_14	C	-3.03377920	-0.38623154	0.53231357	704.9818i, 33.2804, 43.6608, 71.3255, 85.0712, 102.0473, 114.0987, 142.7468, 208.5462, 243.9298, 272.7749, 312.0610, 322.3770, 412.5052, 517.0198, 718.7079, 738.5995, 773.0910, 782.7793, 850.2925, 865.6728, 921.7423, 926.1502, 989.8353, 1029.2543, 1058.1720, 1073.1555, 1092.8685, 1110.2926, 1150.3172, 1177.1599, 1212.5179, 1264.0033, 1290.2568, 1297.9180, 1307.2986, 1329.3461, 1333.0122, 1348.0224, 1365.1075, 1379.2169, 1405.9634, 1410.0920, 1413.3187, 1452.1518, 1480.5726, 1484.8200, 1490.0939, 1497.8794, 1503.7732, 1505.2943, 1512.4582, 1520.8710, 3031.2457, 3032.6942, 3033.3043, 3041.1266, 3050.3909, 3056.6720, 3067.6684, 3069.4638, 3074.3081, 3088.1152, 3094.2832, 3103.1582, 3123.4368, 3132.4650, 3152.6358, 3791.2233
	H	-2.96363154	-0.45611546	1.61800451	
	H	-2.95457051	0.75189143	0.31528871	
	H	-4.02076301	-0.70252281	0.19983833	
	C	-0.52916620	-0.55417446	0.25305458	
	H	-0.50282275	0.52512034	0.08845105	
	H	-0.41137621	-0.70958392	1.33078143	
	C	-1.89307179	-1.07382447	-0.18426413	
	H	-1.95035502	-2.15217800	-0.00157075	
	H	-2.00296342	-0.93810833	-1.26308668	
	C	0.62109938	-1.23058077	-0.48369939	
	H	0.54501679	-1.00072525	-1.55114335	
	H	0.51001020	-2.31472625	-0.39399026	
	C	2.00351349	-0.82592311	0.02048155	
	H	2.76280981	-1.40541201	-0.51170213	
	H	2.09681869	-1.09606917	1.07732056	
	C	2.31672079	0.65759429	-0.14301771	
	H	2.14608920	0.94620532	-1.18401636	
	H	1.62480725	1.25058130	0.45761602	
	C	3.74796689	0.99120502	0.25780194	
H	4.46193348	0.44048229	-0.35637740		
H	3.93073559	0.71996845	1.29875449		
H	3.95973468	2.05411950	0.14733328		
O	-2.87023274	2.07589605	-0.24902160		
H	-3.66931156	2.01151442	-0.79535106		
SP1_15	C	-2.90978517	-0.43564418	0.83476134	705.0305i, 29.0183, 50.8167, 72.5248, 83.1524, 98.1671, 116.2758, 141.5391, 210.8958, 242.6688, 271.1128, 311.1082, 324.9447, 412.7562, 515.9638, 721.5235, 738.5194, 775.2282, 783.4769, 849.8526, 866.3645, 920.1531, 931.7676,
	H	-2.64390518	-0.25117718	1.87577873	
	H	-3.07177836	0.62501616	0.39004287	
	H	-3.86733033	-0.95011487	0.77845505	
	C	-0.50050860	-0.31783340	0.08498712	
	H	-0.67886388	0.68475315	-0.31533671	
	H	-0.19790731	-0.18864555	1.12734403	
C	-1.80567182	-1.10308236	0.04555444		

	H	-1.63761578	-2.11043131	0.44163232	989.4720, 1028.1318, 1057.5906,
	H	-2.12235314	-1.22924149	-0.99260662	1076.2046, 1094.0555, 1111.4978,
	C	0.61548974	-0.99364077	-0.70334169	1158.0056, 1165.7693, 1215.7576,
	H	0.25144705	-1.21021462	-1.71121444	1270.9800, 1282.1190, 1298.2638,
	H	0.84548490	-1.96083159	-0.24481884	1310.1133, 1327.6683, 1338.8440,
	C	1.89392003	-0.16611958	-0.80198089	1344.2385, 1364.9100, 1378.8597,
	H	1.67365563	0.77952606	-1.30707752	1404.8415, 1410.4743, 1413.5942,
	H	2.61329210	-0.69220220	-1.43540319	1453.9964, 1481.4276, 1484.0670,
	C	2.55092534	0.12981647	0.54207191	1490.2667, 1498.1198, 1503.5079,
	H	1.88489878	0.74320449	1.15171784	1505.8963, 1512.8767, 1525.7122,
	H	2.69212904	-0.80877613	1.08593068	3031.0568, 3033.4394, 3034.9088,
	C	3.88851996	0.84161858	0.38488952	3046.9403, 3048.0683, 3056.4828,
	H	3.76278634	1.78593334	-0.14691000	3065.2969, 3068.5979, 3074.3985,
	H	4.58804670	0.23123028	-0.18803132	3087.7457, 3093.0531, 3099.3612,
	H	4.34519202	1.05948829	1.34973797	3123.4178, 3131.6604, 3152.7028,
	O	-3.33055362	1.78421671	-0.42692433	3788.0895
	H	-4.19008635	1.48806092	-0.76549666	
	C	-3.09223255	-0.83574137	0.05015156	708.7981i, 29.5490, 46.8491, 82.8533,
	H	-3.84962949	-1.18037867	0.75178761	90.9816, 112.2556, 128.7171,
	H	-3.31703374	0.28373847	-0.16334011	147.8797, 154.4292, 246.6335,
	H	-3.22618306	-1.32355381	-0.91556291	288.5499, 323.6027, 361.0449,
	C	-0.65035587	-0.37818626	-0.40397626	398.8955, 496.9217, 720.8331,
	H	-0.72537870	-0.92287576	-1.35031294	739.7353, 774.0105, 790.2606,
	H	-0.89976084	0.66333475	-0.62532195	832.9219, 885.2603, 922.6961,
	C	-1.67730311	-0.93144140	0.57579781	934.5305, 986.0185, 1022.1374,
	H	-1.60146217	-0.39288777	1.52359274	1056.4933, 1082.5184, 1096.4795,
	H	-1.44492821	-1.97879398	0.79649496	1108.1527, 1155.9482, 1166.5496,
	C	0.77808109	-0.46234077	0.11740011	1211.8088, 1263.1741, 1280.5090,
	H	1.02832493	-1.50710839	0.33144691	1295.6499, 1314.4807, 1329.6526,
	H	0.83825314	0.07032378	1.06993194	1336.1498, 1352.5962, 1363.9822,
	C	1.79725902	0.10846528	-0.86216857	1378.7752, 1398.1396, 1412.9418,
	H	1.59205657	1.17336890	-1.00961587	1416.2918, 1454.4569, 1480.9096,
	H	1.65575130	-0.36936822	-1.83520810	1484.0571, 1492.2058, 1494.3079,
	C	3.24880316	-0.06882408	-0.42355912	1505.6390, 1509.7702, 1512.8496,
	H	3.46448479	-1.13594312	-0.32281696	1524.3743, 3029.3210, 3032.0016,
	H	3.90482380	0.30449477	-1.21217866	3037.7460, 3043.0626, 3048.0497,
	C	3.58045048	0.64276360	0.88364230	3058.8931, 3065.2872, 3070.0814,
	H	3.03574225	0.21236158	1.72350367	3080.9201, 3086.0140, 3089.7070,
	H	3.31773015	1.70064869	0.82427078	3098.8305, 3125.9332, 3135.7266,
	H	4.64361911	0.57421062	1.11153630	3152.0490, 3787.1109
	O	-3.52519465	1.70898195	-0.12065741	
	H	-4.12306602	1.70840255	0.64332493	
SP1_16	C	2.61481001	-1.04898616	-0.40504440	704.6300i, 31.0364, 48.6237, 66.1501,
	H	2.30105029	-1.39710420	-1.38934288	82.0188, 128.6865, 140.9165,
	H	2.98925455	0.03436389	-0.59232849	149.8144, 201.5240, 276.4768,
	H	3.47272881	-1.62353477	-0.06067290	291.8169, 325.4813, 383.1279,
	C	0.32855615	-0.10655669	0.11062178	409.4117, 505.4628, 719.5559,
	H	0.70505228	0.90211380	-0.08461130	731.7317, 785.1059, 792.1920,
	H	-0.03094151	-0.49417818	-0.84712055	844.8000, 860.0775, 923.6148,
	C	1.48059771	-0.97913685	0.59301263	932.8852, 970.8009, 1032.5090,
	H	1.11264223	-1.99159818	0.79185995	1032.6206, 1077.0009, 1093.2212,
	H	1.85353746	-0.59460679	1.54535783	1117.9283, 1151.0010, 1166.4528,
	C	-0.81954380	-0.04291873	1.11037637	1197.5749, 1262.3698, 1283.6390,
	H	-0.42381264	0.25322443	2.08533347	1294.3533, 1305.1905, 1330.4432,
	H	-1.23598172	-1.04514970	1.24555655	1337.1170, 1362.2667, 1367.4252,
	C	-1.92734163	0.93199987	0.71399662	1386.3577, 1391.3106, 1412.2660,
	H	-1.52457642	1.94793309	0.72744720	1414.4320, 1453.3506, 1479.9943,
	H	-2.71472979	0.89899743	1.47180539	
SP1_17	C	2.61481001	-1.04898616	-0.40504440	704.6300i, 31.0364, 48.6237, 66.1501,
	H	2.30105029	-1.39710420	-1.38934288	82.0188, 128.6865, 140.9165,
	H	2.98925455	0.03436389	-0.59232849	149.8144, 201.5240, 276.4768,
	H	3.47272881	-1.62353477	-0.06067290	291.8169, 325.4813, 383.1279,
	C	0.32855615	-0.10655669	0.11062178	409.4117, 505.4628, 719.5559,
	H	0.70505228	0.90211380	-0.08461130	731.7317, 785.1059, 792.1920,
	H	-0.03094151	-0.49417818	-0.84712055	844.8000, 860.0775, 923.6148,
	C	1.48059771	-0.97913685	0.59301263	932.8852, 970.8009, 1032.5090,
	H	1.11264223	-1.99159818	0.79185995	1032.6206, 1077.0009, 1093.2212,
	H	1.85353746	-0.59460679	1.54535783	1117.9283, 1151.0010, 1166.4528,
	C	-0.81954380	-0.04291873	1.11037637	1197.5749, 1262.3698, 1283.6390,
	H	-0.42381264	0.25322443	2.08533347	1294.3533, 1305.1905, 1330.4432,
	H	-1.23598172	-1.04514970	1.24555655	1337.1170, 1362.2667, 1367.4252,
	C	-1.92734163	0.93199987	0.71399662	1386.3577, 1391.3106, 1412.2660,
	H	-1.52457642	1.94793309	0.72744720	1414.4320, 1453.3506, 1479.9943,
	H	-2.71472979	0.89899743	1.47180539	

	C	-2.55029582	0.66327781	-0.65583991	1482.1550, 1495.0762, 1497.6167,
	H	-3.34617130	1.39092437	-0.82453641	1502.4482, 1506.7376, 1517.1916,
	H	-1.80938947	0.83890322	-1.43864259	1524.0221, 3030.3336, 3038.1945,
	C	-3.11568439	-0.74553786	-0.79429686	3043.8519, 3048.4515, 3055.8527,
	H	-3.81928399	-0.96176508	0.01195874	3060.1947, 3065.4466, 3073.5507,
	H	-2.32727889	-1.49805785	-0.75400564	3081.9282, 3088.0905, 3094.1962,
	H	-3.64117859	-0.86975877	-1.74043703	3097.3099, 3122.3451, 3131.2204,
	O	3.50562962	1.37805528	-0.51643130	3152.6669, 3788.4836
	H	4.32745233	1.15200267	-0.05312825	
SP1_18	C	2.22917392	-1.32635067	0.00162737	703.5861i, 30.4315, 46.8614, 65.2273,
	H	2.03783771	-1.79945361	-0.96189580	75.3250, 94.7758, 151.2540, 204.0684,
	H	3.09489568	-0.58316187	-0.21419614	211.4074, 250.7211, 291.4842,
	H	2.61202177	-2.05971540	0.70898476	312.2468, 332.7974, 429.3757,
	C	0.58742435	0.52503763	-0.48121792	528.3823, 715.6774, 739.8630,
	H	1.44811988	1.13532200	-0.76338504	779.4073, 786.3985, 852.2592,
	H	0.25057955	0.02785124	-1.39505198	871.6422, 890.4191, 943.8285,
	C	1.05104145	-0.53007820	0.51690948	966.8149, 1046.5393, 1051.6612,
	H	0.23093989	-1.21912731	0.74326360	1063.3311, 1072.7593, 1121.2616,
	H	1.31665697	-0.04626592	1.46085030	1146.5062, 1176.3670, 1207.8184,
	C	-0.51539264	1.43499281	0.05678364	1251.6649, 1290.5024, 1295.5357,
	H	-0.80305811	2.14004107	-0.72726220	1317.8214, 1323.5123, 1336.7439,
	H	-0.10944909	2.03373775	0.87622403	1346.3723, 1365.1929, 1391.7418,
	C	-1.76473752	0.70421486	0.54702071	1399.9387, 1410.7835, 1412.6117,
	H	-2.49878096	1.44413470	0.87687891	1453.1295, 1479.2885, 1487.1954,
	H	-1.52563853	0.10532470	1.43069814	1493.6383, 1498.4393, 1503.7077,
	C	-2.40913340	-0.19363920	-0.50302090	1504.3569, 1513.9618, 1523.7803,
	H	-2.57943292	0.38570734	-1.41495585	3034.5361, 3039.8637, 3046.0192,
H	-1.71989133	-0.99655381	-0.77540617	3048.5563, 3051.0961, 3056.7826,	
C	-3.72150077	-0.79735524	-0.01984885	3067.1985, 3069.5512, 3081.7555,	
H	-4.44313534	-0.01514803	0.21959582	3086.7127, 3092.0751, 3098.3183,	
H	-3.56493325	-1.38847573	0.88389074	3122.5829, 3131.4988, 3151.4301,	
H	-4.16796153	-1.44737714	-0.77154174	3790.7949	
O	4.13396406	0.41592141	-0.18351055		
H	4.60826470	0.05485681	0.58187177		
SP1_19	C	-2.52900665	-0.15992988	-0.57922419	786.7960i, 40.2819, 50.4378, 66.9085,
	H	-3.17543342	-0.51124881	0.22553661	109.8244, 146.9501, 150.9182,
	H	-2.19675762	0.90782940	-0.23497444	187.8692, 241.7883, 288.1460,
	H	-3.11788434	0.04862760	-1.47030333	300.8076, 352.3701, 371.8210,
	C	-0.63626154	-1.54306479	0.42458002	441.0731, 519.2446, 680.9392,
	H	-1.34841509	-2.07670068	1.05893859	732.6232, 765.8459, 809.0907,
	H	0.13375528	-2.26793517	0.15384694	863.9864, 878.6718, 898.1773,
	C	-1.35841857	-1.08453527	-0.84085889	947.0605, 962.6502, 1001.3274,
	H	-1.73673722	-1.96793607	-1.36353298	1030.5621, 1056.5927, 1071.9222,
	H	-0.65659219	-0.61102305	-1.53169702	1085.1875, 1128.1174, 1156.7670,
	C	-0.01122285	-0.40973054	1.23826660	1165.1284, 1233.0448, 1243.8867,
	H	0.48640169	-0.83841855	2.11163791	1279.3514, 1311.1269, 1322.6244,
	H	-0.80545998	0.23128163	1.62925415	1327.7323, 1345.8070, 1372.0576,
	C	1.00349924	0.43434207	0.46670789	1389.6402, 1401.6313, 1408.7751,
	H	1.36387988	1.23842502	1.11552075	1414.0629, 1448.5159, 1478.8396,
	H	0.52602006	0.92050088	-0.39098560	1492.4212, 1497.1338, 1500.9902,
	C	2.20291980	-0.35652691	-0.04579875	1504.1040, 1507.2385, 1514.7630,
	H	2.64351793	-0.91528600	0.78444011	1536.5656, 3028.6644, 3043.4595,
H	1.86805562	-1.09876307	-0.77373034	3047.5389, 3049.3353, 3056.2470,	
C	3.25487802	0.54005910	-0.68549507	3057.5535, 3063.5156, 3075.5379,	
H	3.63553655	1.26607163	0.03408459	3081.3673, 3088.8941, 3091.3072,	
H	2.83140301	1.09633887	-1.52308438	3100.5343, 3123.9338, 3133.4492,	
H	4.09999649	-0.03616827	-1.05996137	3155.7592, 3786.7750	
O	-1.89224147	2.25023418	0.12272473		

	H	-0.97167962	2.08884855	0.38414640	
SP1_20	C	-2.62815014	0.41386578	-0.28497814	756.2548i, 39.1288, 57.7330, 81.3910, 104.2152, 135.1724, 145.8328, 211.4362, 227.1695, 260.9891, 307.6478, 347.9428, 365.6749, 445.1855, 503.4794, 660.7962, 740.0219, 764.4722, 823.7879, 858.0421, 866.2729, 910.3981, 957.3182, 966.5756, 1011.5042, 1047.5394, 1063.1888, 1095.0432, 1117.2129, 1125.8134, 1159.3820, 1179.1130, 1228.1936, 1255.4114, 1288.5411, 1300.5486, 1332.1612, 1334.4468, 1348.5163, 1385.2460, 1386.1081, 1395.6580, 1409.6814, 1416.7999, 1440.0241, 1484.9366, 1489.7880, 1492.1764, 1495.6660, 1506.3882, 1509.8740, 1513.6139, 1514.6231, 3030.8160, 3038.5173, 3042.4724, 3050.9719, 3052.9611, 3060.1805, 3062.9410, 3075.8186, 3083.6507, 3085.6252, 3095.1250, 3100.3147, 3127.4979, 3139.5887, 3154.9552, 3780.6383
	H	-3.51246287	0.87546408	0.14954257	
	H	-1.85093456	1.28361978	-0.29877197	
	H	-2.79819339	0.18941569	-1.33870991	
	C	-1.03884298	-1.58066034	-0.20622228	
	H	-0.77803771	-2.44690051	0.40744696	
	H	-1.45162244	-1.97488144	-1.13831053	
	C	-2.13326657	-0.78206803	0.50188850	
	H	-1.79987698	-0.46084482	1.49101584	
	H	-2.98253608	-1.44761974	0.68112309	
	C	0.23247203	-0.79483369	-0.52405642	
	H	-0.00966479	0.06956835	-1.14973066	
	H	0.88818048	-1.42923274	-1.12267352	
	C	0.98904656	-0.32867129	0.71712484	
	H	1.32558034	-1.20541423	1.27973027	
	H	0.31015291	0.20351315	1.39129631	
	C	2.19152127	0.56223642	0.40697557	
	H	1.85543282	1.45239524	-0.13411125	
H	2.62487316	0.91412336	1.34493288		
C	3.26856003	-0.14013786	-0.41260226		
H	2.91075731	-0.39421865	-1.40962558		
H	3.58302506	-1.06437192	0.07566358		
H	4.14719452	0.49274945	-0.52986345		
O	-0.93384237	2.36973802	-0.15747264		
H	-0.27917006	1.88634479	0.37204768		
SP1_21	C	-2.66087316	0.28040903	0.59717024	777.6506i, 34.0176, 61.6505, 72.6272, 80.5689, 123.0532, 150.4969, 172.6561, 206.0092, 270.6600, 310.5151, 321.9882, 347.2081, 463.3607, 468.1758, 663.1620, 752.8779, 778.3150, 824.2606, 842.7817, 884.4929, 915.2436, 950.9198, 983.4330, 1017.4212, 1037.2344, 1076.3038, 1102.4980, 1113.0943, 1134.2665, 1169.0919, 1212.2983, 1241.0831, 1259.3543, 1289.8418, 1312.3769, 1320.0216, 1336.7632, 1339.2154, 1377.6674, 1382.9237, 1392.9865, 1409.8201, 1416.7105, 1434.3509, 1480.5895, 1487.1238, 1491.7778, 1493.6768, 1501.6466, 1506.0944, 1513.3390, 1516.7807, 3001.5196, 3037.1667, 3041.2184, 3042.9025, 3048.1470, 3057.8292, 3070.5223, 3073.6693, 3079.7232, 3086.8527, 3087.9857, 3103.1282, 3124.7648, 3134.4034, 3154.8534, 3784.7323
	H	-2.38711238	0.17264868	1.64740016	
	H	-2.10837526	1.24361922	0.24059038	
	H	-3.71074493	0.55180773	0.50662749	
	C	-0.89491582	-1.48260362	0.05701745	
	H	-0.85589530	-1.80233050	1.10290857	
	H	-0.73254355	-2.37924104	-0.54608172	
	C	-2.28328710	-0.92323368	-0.24260070	
	H	-3.02435270	-1.70906358	-0.07212813	
	H	-2.35675159	-0.66526664	-1.30292775	
	C	0.23874202	-0.49723187	-0.19961544	
	H	0.11306106	0.37369967	0.44682448	
	H	0.17764315	-0.14114135	-1.23690928	
	C	1.61811957	-1.10352619	0.03080455	
	H	1.70335159	-2.02481127	-0.55123428	
	H	1.70655898	-1.39274869	1.08274555	
	C	2.76840416	-0.16793506	-0.33361714	
	H	3.71278678	-0.69619839	-0.19081715	
H	2.70909050	0.07259118	-1.39864794		
C	2.78507798	1.12197120	0.47978706		
H	2.78836396	0.90362213	1.54933826		
H	1.91316437	1.74275886	0.27280045		
H	3.67070325	1.71582350	0.25716672		
O	-1.48500325	2.35504009	-0.40132540		
H	-0.86652770	1.82681083	-0.93072878		
SP1_22	C	-2.50107655	-0.69231896	-0.18052239	779.4740i, 48.3290, 68.8382, 76.4030, 120.3053, 144.2011, 165.4538, 203.8402, 235.6797, 301.4576, 342.2637, 358.6922, 394.8715, 448.4002, 525.1933, 687.7068, 720.8363, 769.1763, 816.3922,
	H	-2.84466227	-1.03641514	0.79535790	
	H	-2.43083481	0.46981820	-0.07443570	
	H	-3.29029045	-0.81344348	-0.92011613	
	C	-0.13604153	-1.35742315	0.50442106	
	H	-0.52866733	-1.93965232	1.34179103	
H	0.74245994	-1.89667995	0.14270026		

	C	-1.18904103	-1.32102457	-0.60180257	848.4492, 877.6578, 894.5299,
	H	-1.39298735	-2.34745291	-0.92032355	951.1562, 960.7683, 1007.3441,
	H	-0.79882829	-0.80889220	-1.48454875	1009.4659, 1054.0446, 1067.1023,
	C	0.28492810	0.01888118	1.01721836	1085.7577, 1127.8694, 1152.9892,
	H	1.02850119	-0.11003961	1.80599699	1165.1975, 1224.2305, 1235.3942,
	H	-0.57084289	0.50030298	1.49788333	1278.2851, 1302.9616, 1322.1257,
	C	0.85304630	0.94031830	-0.06479418	1335.9649, 1362.2983, 1376.0836,
	H	1.14889545	1.88588413	0.39917388	1385.3976, 1403.9611, 1404.8313,
	H	0.07741792	1.18154968	-0.79707985	1416.8585, 1448.0882, 1477.1129,
	C	2.05409284	0.36372642	-0.81566178	1487.6287, 1495.9227, 1502.1095,
	H	1.73983623	-0.50525694	-1.39879806	1505.9837, 1511.0970, 1519.0717,
	H	2.39804543	1.10434276	-1.53949249	1541.9387, 3038.2563, 3043.8373,
	C	3.20943861	-0.02626485	0.09886135	3051.9700, 3054.2994, 3058.5816,
	H	2.94141420	-0.85770466	0.75125661	3061.4384, 3074.7736, 3076.4155,
	H	3.50067853	0.81225465	0.73420080	3085.6604, 3090.6888, 3096.2743,
	H	4.08260294	-0.32881181	-0.47771204	3097.6245, 3124.0357, 3134.3943,
	O	-2.46603954	1.89059472	0.02071408	3154.8228, 3788.1698
	H	-1.52650253	2.01007262	0.23211409	
	C	-2.76591744	0.12909484	-0.46133831	
	H	-3.80908772	0.38591924	-0.28751487	769.9379i, 37.0006, 59.7483, 89.5052,
	H	-2.22881784	1.15975832	-0.36911058	103.8788, 116.7278, 132.3329,
	H	-2.62079434	-0.18165358	-1.49656801	199.9426, 207.6564, 278.9906,
	C	-0.86986873	-1.46014407	0.16292708	306.2777, 314.4879, 336.6965,
	H	-0.57474654	-2.19256163	0.91856679	461.3540, 473.5965, 672.8356,
	H	-0.97121651	-2.01060029	-0.77727756	752.7642, 778.8243, 828.2623,
	C	-2.22314075	-0.86625154	0.54409180	847.6524, 878.8769, 911.5389,
	H	-2.15434015	-0.38856819	1.52515574	954.7119, 978.7295, 1019.8155,
	H	-2.94613488	-1.67930611	0.65299413	1035.1576, 1076.7115, 1103.3090,
	C	0.24344028	-0.42977382	0.01354563	1113.8631, 1134.6328, 1176.9394,
	H	0.28042608	0.18193252	0.92185643	1205.3117, 1245.6418, 1258.6337,
	H	0.01580782	0.24109073	-0.82168633	1293.4857, 1302.2777, 1323.6698,
	C	1.60766718	-1.06712994	-0.22674386	1329.1884, 1334.5268, 1378.1189,
	H	1.51914515	-1.78758004	-1.04409807	1384.5948, 1389.6811, 1407.0880,
	H	1.89437580	-1.64025495	0.66036734	1415.0279, 1436.1218, 1480.3669,
	C	2.70843981	-0.06295553	-0.55910637	1486.9131, 1492.5725, 1493.5038,
	H	3.63643493	-0.60508231	-0.74902644	1505.2940, 1506.9987, 1511.2617,
	H	2.45482466	0.45026587	-1.49033457	1520.6278, 3020.2392, 3037.6536,
	C	2.94358913	0.96707044	0.54032452	3042.6587, 3045.0777, 3049.9225,
	H	3.12736745	0.47689855	1.49827601	3056.2987, 3058.8928, 3073.3290,
	H	2.08380666	1.62591969	0.66481850	3079.9987, 3086.1804, 3089.6714,
	H	3.80415043	1.59543119	0.31470262	3094.7821, 3124.1558, 3133.3137,
	O	-1.57947892	2.39007730	-0.05329910	3154.9081, 3788.1530
	H	-0.74062652	1.98831028	0.22306868	
	C	2.30175218	-0.34601463	0.95666208	
	H	3.32672417	-0.56727471	1.24778533	765.9990i, 42.1931, 61.1492, 95.8332,
	H	2.39569022	0.70441693	0.46089810	120.6099, 130.0940, 165.4096,
	H	1.68262797	-0.19229304	1.84161573	186.5758, 251.0939, 276.2377,
	C	0.21295115	-1.24831604	-0.19243199	307.1733, 326.6223, 358.0636,
	H	-0.13425028	-2.05553700	-0.84327663	445.1009, 529.7162, 672.0606,
	H	-0.27097943	-1.40314674	0.77614550	739.7633, 798.5819, 817.0170,
	C	1.72332903	-1.36373927	-0.00597025	845.4914, 867.4919, 910.7846,
	H	2.22573130	-1.27629812	-0.97320742	949.4403, 973.1060, 1011.7742,
	H	1.95621915	-2.36470253	0.36741942	1042.8549, 1062.3256, 1096.8308,
	C	-0.23717429	0.08637758	-0.77687715	1122.0463, 1133.9922, 1168.0314,
	H	0.33743794	0.28236600	-1.68916040	1195.5111, 1240.7879, 1258.9091,
	H	-0.00353626	0.89076021	-0.07418310	1286.0382, 1309.7528, 1319.7255,
	C	-1.72572434	0.13033021	-1.12088204	1329.0668, 1340.8514, 1378.0248,
	H	-1.92509874	-0.58308787	-1.92454640	1386.6917, 1390.1508, 1406.3722,

	H	-1.96844105	1.12043469	-1.51533286	1415.6612, 1437.5760, 1480.3583,
	C	-2.65273196	-0.17222803	0.05665069	1485.8155, 1495.6981, 1498.3068,
	H	-3.68565283	-0.07640161	-0.28235427	1504.7162, 1509.5285, 1510.6079,
	H	-2.53131865	-1.21303378	0.36427192	1525.0821, 3022.5751, 3040.9563,
	C	-2.42528391	0.74438382	1.25320458	3045.5337, 3046.2130, 3055.6093,
	H	-2.48803282	1.79299527	0.95661410	3061.3388, 3066.7662, 3072.9205,
	H	-1.44174014	0.58669857	1.69792470	3081.1742, 3086.5421, 3093.8131,
	H	-3.16861090	0.57064649	2.03016752	3096.1656, 3122.5289, 3132.7872,
	O	2.58343912	1.88488882	-0.31756417	3153.3122, 3787.1692
	H	1.84301020	1.71958477	-0.92240345	
SP1_25	C	-2.64790613	-0.54660101	0.77080106	763.8030i, 45.7240, 66.4379, 78.0457,
	H	-2.15173572	-0.62973113	1.73840620	108.7716, 117.8785, 141.6097,
	H	-2.69728824	0.59623773	0.54859166	158.8376, 245.7948, 277.0502,
	H	-3.69745085	-0.81991460	0.86065534	288.3031, 296.5707, 330.7238,
	C	-0.41251503	-1.14491203	-0.30320254	416.8618, 545.0880, 671.2865,
	H	-0.04090282	-1.52851034	0.65031878	739.3716, 786.4394, 818.5459,
	H	0.02714181	-1.77263742	-1.08329229	850.3894, 875.8565, 908.6840,
	C	-1.93092794	-1.29741652	-0.33303510	950.2315, 974.4394, 1034.8462,
	H	-2.17929557	-2.35878115	-0.24594701	1054.1150, 1066.8484, 1089.9268,
	H	-2.31739602	-0.97424125	-1.30354573	1118.7817, 1134.3915, 1177.0204,
	C	0.06776370	0.29027787	-0.49806682	1202.3374, 1245.6514, 1260.5209,
	H	-0.23792413	0.89758201	0.35965533	1297.7961, 1304.5969, 1324.4853,
	H	-0.42757843	0.70579344	-1.38315472	1326.2085, 1336.5694, 1351.9252,
	C	1.57880948	0.41416449	-0.67685481	1388.1195, 1404.2459, 1405.4664,
	H	1.83256117	1.45955776	-0.87126368	1412.8103, 1438.7833, 1481.3466,
	H	1.88512836	-0.14713601	-1.56514621	1487.7201, 1493.4562, 1498.0952,
	C	2.38639840	-0.07073775	0.52252762	1503.5841, 1510.7317, 1512.3797,
H	2.01964251	0.42614131	1.42524036	1514.6228, 3017.0266, 3036.1056,	
H	2.22301997	-1.13994635	0.67011280	3041.2835, 3046.7106, 3049.1648,	
C	3.87717321	0.19409749	0.35621947	3057.9060, 3060.6212, 3069.7598,	
H	4.07182874	1.26191220	0.24786846	3073.3140, 3086.3151, 3093.2540,	
H	4.26069781	-0.30343771	-0.53580013	3096.3120, 3124.6781, 3133.5985,	
H	4.44769745	-0.16601175	1.21145526	3154.4464, 3791.1481	
O	-2.81505870	1.94151865	0.08749153		
H	-2.01045056	1.92773876	-0.45441998		
SP1_26	C	-2.42104887	-0.49511151	0.34268964	677.9125i, 36.6065, 40.8135, 60.2137,
	H	-2.40587052	-0.46060861	1.43250099	78.7383, 94.7022, 116.0469, 138.9587,
	H	-3.53359773	-0.59439828	0.02569403	166.1753, 242.5368, 250.6331,
	H	-1.95417806	-1.41478433	-0.00573122	335.3495, 352.9169, 395.4903,
	C	-0.43074093	1.06973834	0.15936799	495.8595, 726.4335, 741.1564,
	H	-0.12118798	2.02022704	-0.28280415	748.3565, 782.7995, 843.9485,
	H	-0.41661891	1.21431984	1.24400771	902.7011, 930.8447, 954.4558,
	C	-1.86076156	0.76141604	-0.29069554	981.8664, 1032.2029, 1050.1986,
	H	-1.88368641	0.66132847	-1.37799333	1077.1639, 1091.8980, 1102.1777,
	H	-2.50598194	1.60502646	-0.04091705	1147.6842, 1189.3650, 1226.2967,
	C	0.58236872	-0.00505728	-0.21689305	1245.8820, 1265.4396, 1294.7804,
	H	0.51153968	-0.20781656	-1.29062199	1300.5526, 1329.4848, 1333.8270,
	H	0.33676490	-0.94240872	0.28956115	1342.0675, 1350.6468, 1380.1752,
	C	2.01340016	0.38394200	0.13046446	1396.7057, 1411.0307, 1415.6637,
	H	2.07951918	0.60222134	1.20116412	1457.2451, 1484.8939, 1487.1075,
	H	2.27209739	1.31342744	-0.38642817	1494.4741, 1496.6722, 1503.8847,
	C	3.03311196	-0.68987527	-0.22702992	1505.3267, 1514.5156, 1524.8499,
H	2.77492447	-1.61624861	0.29254426	3030.0416, 3034.1125, 3043.1226,	
H	2.96306287	-0.90823094	-1.29574586	3049.8409, 3055.8179, 3057.4344,	
C	4.45858203	-0.28361800	0.12304631	3059.0654, 3070.1596, 3082.5770,	
H	4.55375603	-0.08677292	1.19185996	3085.0747, 3094.0583, 3101.7361,	
H	4.74288095	0.62684663	-0.40645632	3123.4708, 3132.0688, 3152.7785,	
H	5.17511976	-1.06111711	-0.13937942		

	O	-4.95472854	-0.57135472	-0.16818244	3790.9977
	H	-5.20018433	-0.62877933	0.76850548	
SP1_27	C	-2.43334255	-0.33620620	0.55425857	680.1257i, 34.5346, 44.3957, 56.7366, 72.8022, 95.2999, 116.7779, 137.6581, 157.0445, 248.8699, 257.6526, 320.6723, 362.6087, 395.4118, 496.3780, 725.0297, 734.6732, 758.0786, 808.4725, 844.8989, 890.8785, 920.5509, 940.2045, 995.8357, 1022.7722, 1051.4333, 1080.0292, 1095.5701, 1102.0094, 1147.9821, 1176.2689, 1227.2830, 1256.0247, 1265.9501, 1292.6426, 1306.7968, 1328.1744, 1333.2744, 1344.3186, 1348.3350, 1377.4723, 1395.2012, 1409.2414, 1414.1274, 1456.5549, 1484.5106, 1487.2518, 1494.3218, 1496.5673, 1503.6726, 1505.2344, 1514.5126, 1521.3605, 3029.3289, 3033.6125, 3043.1470, 3049.1038, 3055.5440, 3057.5830, 3058.5664, 3069.7039, 3082.6747, 3085.3069, 3094.3590, 3102.0605, 3123.7731, 3132.0121, 3152.3507, 3788.8118
	H	-2.38648653	-0.15119566	1.62794161	
	H	-3.56668909	-0.43066573	0.32184137	
	H	-1.98890048	-1.30328178	0.32554501	
	C	-0.42082148	1.13664360	0.08115377	
	H	-0.10923352	2.00633771	-0.50305428	
	H	-0.36310997	1.43399828	1.13256565	
	C	-1.87264141	0.80350977	-0.27051732	
	H	-1.93921876	0.55192102	-1.33142827	
	H	-2.49055150	1.68993926	-0.12075714	
	C	0.55614773	-0.00569417	-0.17138425	
	H	0.44057592	-0.35905024	-1.20149656	
	H	0.31301408	-0.85399071	0.47418982	
	C	2.00672345	0.39422787	0.06508649	
	H	2.11746409	0.76449871	1.08926279	
	H	2.26327125	1.23178877	-0.59115929	
	C	2.99124159	-0.74505469	-0.16607231	
H	2.73627064	-1.57832523	0.49382254		
H	2.87559623	-1.11640317	-1.18763259		
C	4.43672266	-0.32668149	0.06883292		
H	4.57660490	0.02488436	1.09204551		
H	4.71797724	0.48725163	-0.60086166		
H	5.12744212	-1.15224242	-0.09898789		
O	-4.89637473	-0.65393689	-0.16943288		
H	-4.73720883	-1.53843778	-0.53452081		
SP1_28	C	2.84889829	-0.51234157	0.28095469	669.3379i, 32.8728, 48.6815, 67.5228, 85.4454, 101.5864, 112.5456, 127.6190, 209.0293, 244.2264, 267.7398, 288.2002, 337.4025, 407.4263, 509.1576, 725.3290, 729.1731, 751.3386, 791.5148, 850.6178, 892.1821, 916.9232, 960.4879, 986.2747, 1041.8476, 1057.7959, 1065.2000, 1081.8729, 1105.9949, 1141.8195, 1192.7486, 1236.9855, 1244.8949, 1271.7168, 1292.9723, 1300.9419, 1327.8952, 1331.1175, 1337.4919, 1355.9552, 1376.1785, 1394.8287, 1409.3838, 1413.1588, 1456.1852, 1482.9307, 1486.7389, 1490.2409, 1501.5098, 1503.3998, 1504.9012, 1512.7692, 1521.6104, 3029.9145, 3037.8934, 3039.8588, 3048.6599, 3057.4178, 3059.9838, 3063.1899, 3073.5285, 3077.8852, 3082.6159, 3094.6583, 3106.8463, 3123.4144, 3132.6803, 3147.2188, 3791.6110
	H	3.29420568	-1.39167737	-0.18391489	
	H	3.51779555	0.37502167	-0.05578297	
	H	2.93986075	-0.58204809	1.36480549	
	C	0.48535216	-1.37940092	0.23165755	
	H	0.90126340	-2.32781776	-0.11763909	
	H	0.44930135	-1.44087488	1.32364274	
	C	1.43038338	-0.24730549	-0.17339924	
	H	1.08620453	0.69610331	0.25236766	
	H	1.40677551	-0.12875605	-1.25942071	
	C	-0.93138732	-1.22051049	-0.31436157	
	H	-1.51939249	-2.09856707	-0.03426401	
	H	-0.89729758	-1.20965317	-1.40810653	
	C	-1.65220807	0.03013205	0.17541504	
	H	-1.13842393	0.92454089	-0.18640316	
	H	-1.60677980	0.06993906	1.26912469	
	C	-3.10835275	0.08552767	-0.27019593	
H	-3.15034929	0.02613673	-1.36091764		
H	-3.63184030	-0.79751942	0.10511477		
C	-3.81904913	1.34615242	0.20423289		
H	-3.32766205	2.23831348	-0.18640405		
H	-3.80527088	1.41188469	1.29315587		
H	-4.85910330	1.36800461	-0.11924959		
O	4.28084978	1.57080880	-0.26887240		
H	4.57209525	1.68697710	0.64905009		
SP1_29	C	-2.41810532	-0.49481317	0.55342393	751.3385i, 38.3298, 49.0664, 63.6819, 70.3330, 96.3304, 117.2968, 137.8313, 160.5261, 246.5953, 256.3023, 337.7923, 362.0234, 385.9025, 490.9377, 702.4159, 729.3368,
	H	-2.36711260	-0.35707216	1.63385289	
	H	-3.55201742	-0.64348611	0.33640779	
	H	-1.95195995	-1.43656946	0.27057511	
	C	-0.45497094	1.06429615	0.14474173	
	H	-0.17357042	1.97093459	-0.39701984	

	H	-0.40204662	1.31123971	1.20925418	750.6640, 782.0469, 843.8666,
	C	-1.89756093	0.70212539	-0.21499487	904.6940, 934.0297, 951.5215,
	H	-1.95596762	0.50250992	-1.28883278	975.6154, 1025.5957, 1049.4250,
	H	-2.54021024	1.56203471	-0.01647335	1079.6443, 1092.6887, 1102.5645,
	C	0.55503783	-0.03382845	-0.16699395	1146.5838, 1181.3928, 1232.1966,
	H	0.44534785	-0.34020623	-1.21267694	1258.6539, 1289.2117, 1301.5518,
	H	0.34069533	-0.91945935	0.43705211	1327.1305, 1331.9469, 1335.8632,
	C	1.99361114	0.39929122	0.08375831	1350.3145, 1355.6871, 1389.8832,
	H	2.09793271	0.72210396	1.12452987	1395.3611, 1410.6492, 1414.6660,
	H	2.22087167	1.27562154	-0.53141431	1448.4586, 1485.2314, 1487.1884,
	C	3.01160730	-0.69613391	-0.20672690	1489.0414, 1494.7659, 1502.9151,
	H	2.78579285	-1.56832008	0.41210951	1504.4729, 1507.8819, 1514.7444,
	H	2.90244810	-1.02026601	-1.24492780	3029.2203, 3034.0080, 3043.4254,
	C	4.44451363	-0.24478005	0.04357245	3045.0706, 3049.2470, 3056.8857,
	H	4.57876114	0.05915399	1.08266761	3057.2176, 3070.0265, 3083.2346,
	H	4.69667665	0.61016867	-0.58538752	3086.8054, 3088.9512, 3097.3174,
	H	5.15965694	-1.03879429	-0.16818338	3122.9475, 3132.4439, 3158.4550,
	O	-4.87936767	-0.59321781	-0.18500393	3787.9761
	H	-4.65515324	-0.12079405	-1.00218585	
	C	-2.88239360	-0.66185209	0.20480692	
	H	-2.95536105	-0.88313187	1.26940233	670.7644i, 30.5487, 40.6581, 55.9382,
	H	-3.79509707	0.00421008	-0.06352269	66.9147, 94.8085, 128.9915, 137.8193,
	H	-3.02390155	-1.57533185	-0.37240243	148.0747, 233.1325, 283.0238,
	C	-0.36193944	-0.73376033	0.14485960	323.4844, 362.5684, 389.2841,
	H	-0.34527877	-0.99342348	1.20779980	493.0174, 725.9729, 732.6229,
	H	-0.40676605	-1.68029317	-0.40195199	756.8929, 784.0869, 844.1892,
	C	-1.61672750	0.08390824	-0.15626419	891.2238, 939.0028, 961.8394,
	H	-1.63278219	0.34338205	-1.21690717	983.7238, 1032.3626, 1052.7747,
	H	-1.57544531	1.02633037	0.39413629	1068.1455, 1080.9470, 1106.8678,
	C	0.92367423	0.00021603	-0.21591188	1139.5808, 1197.4074, 1229.6597,
	H	0.94945536	0.95228860	0.31993103	1247.0651, 1259.4217, 1295.2610,
	H	0.91320063	0.24644863	-1.28274170	1304.8523, 1328.1583, 1333.0681,
	C	2.17445340	-0.81143278	0.10209048	1333.7895, 1359.1496, 1379.8013,
	H	2.08387235	-1.79542935	-0.36553612	1390.2317, 1406.2458, 1415.9093,
	H	2.22212483	-0.98642369	1.18165543	1456.3726, 1483.0626, 1485.7647,
	C	3.47396136	-0.15553393	-0.35862846	1493.6631, 1498.0292, 1505.0857,
	H	4.30432980	-0.83407165	-0.15453126	1511.8477, 1513.2909, 1519.2098,
	H	3.44289680	-0.02404181	-1.44347418	3031.6283, 3034.4802, 3043.4352,
	C	3.74735305	1.18768651	0.30915658	3049.4105, 3058.4010, 3059.0790,
	H	3.72551659	1.08973545	1.39621760	3062.4552, 3071.7748, 3084.0822,
	H	3.00479948	1.93381234	0.02783028	3085.8485, 3092.4188, 3102.2936,
	H	4.72574470	1.57566431	0.02803738	3125.5533, 3135.2068, 3148.0782,
	O	-4.89741848	0.91357501	-0.18001982	3791.8465
	H	-5.20824962	0.83628509	0.73556176	
	C	2.87755346	-0.62337006	0.31708500	
	H	3.04691114	-1.46397135	-0.35550209	669.1682i, 36.1487, 37.4524, 54.3166,
	H	3.78548650	0.09074270	0.19780571	89.8135, 94.9194, 126.4256, 136.9004,
	H	2.92291237	-0.96343895	1.35145501	150.3281, 233.0520, 281.7808,
	C	0.36288315	-0.71905645	0.14787037	325.0494, 362.7122, 389.6550,
	H	0.44494953	-1.59512533	-0.50248263	492.3847, 724.5146, 733.8127,
	H	0.30943343	-1.10056732	1.17202183	753.6747, 782.6262, 846.3453,
	C	1.61419691	0.14372886	-0.00540597	888.4377, 934.9820, 967.6281,
	H	1.53554754	1.01408137	0.64937709	983.7243, 1030.4977, 1053.1655,
	H	1.66696297	0.52641424	-1.02699891	1068.1569, 1081.3528, 1107.3408,
	C	-0.92023411	0.03546172	-0.17788142	1140.2650, 1193.8924, 1236.0046,
	H	-0.87279093	0.40304713	-1.20821544	1244.1006, 1260.4614, 1290.5449,
	H	-0.98273797	0.91907073	0.46204397	1310.2051, 1326.4968, 1329.3297,
	C	-2.16811110	-0.82334081	-0.00572599	1337.0078, 1359.3085, 1379.2477,
SP1_30					
SP1_31					

	H	-2.25706286	-1.11799423	1.04477860	1390.1727, 1406.8703, 1415.1538,
	H	-2.04030989	-1.74801080	-0.57482806	1455.5979, 1483.2397, 1485.0672,
	C	-3.45922049	-0.13822500	-0.44681020	1492.8038, 1497.7321, 1504.9286,
	H	-3.38531311	0.11426749	-1.50793928	1511.3474, 1512.6230, 1519.8021,
	H	-4.28455742	-0.84683206	-0.35579318	3031.5868, 3034.1900, 3043.0690,
	C	-3.78523613	1.11794257	0.35364325	3048.7917, 3058.2739, 3058.8424,
	H	-3.04453197	1.90036071	0.19112260	3062.6187, 3071.3219, 3083.2742,
	H	-3.80866370	0.89894113	1.42285718	3085.6276, 3092.2158, 3102.1731,
	H	-4.75730699	1.52240964	0.07385133	3125.4336, 3135.7272, 3147.4455,
	O	4.90908422	0.90259279	-0.16908331	3789.8860
	H	5.31740746	0.26701755	-0.77753750	
SP1_32	C	2.64576043	-0.72498495	0.40771287	670.9077i, 27.7094, 45.7828, 69.2574,
	H	2.50317131	-1.65412063	-0.14364295	81.7232, 109.1928, 122.3721,
	H	3.72480510	-0.36109823	0.17991621	124.8562, 204.4389, 243.5459,
	H	2.63937350	-0.92670487	1.47868222	271.6798, 303.8742, 323.7689,
	C	0.22412380	-0.02777469	0.28781481	396.6896, 515.5898, 725.4890,
	H	-0.00243240	-0.96568189	-0.22513163	728.7972, 751.5449, 793.3581,
	H	0.10782256	-0.22398141	1.35858642	851.1383, 870.7587, 929.4478,
	C	1.67356759	0.35903164	-0.00223117	963.6697, 990.9752, 1032.2535,
	H	1.91293079	1.28556206	0.52372187	1055.1959, 1065.4472, 1075.1351,
	H	1.78475778	0.56898075	-1.06837449	1108.5885, 1141.9239, 1190.0259,
	C	-0.76301337	1.05371508	-0.13871998	1238.1361, 1248.2264, 1268.9469,
	H	-0.70292733	1.18384351	-1.22367742	1286.4979, 1309.0512, 1327.0052,
	H	-0.45360289	2.00469962	0.30235304	1328.6539, 1341.1092, 1344.1355,
	C	-2.20868003	0.76500207	0.25588802	1377.3336, 1401.0649, 1404.7928,
	H	-2.83254678	1.61737135	-0.02623428	1412.9386, 1455.4531, 1482.7651,
	H	-2.27741346	0.68246942	1.34527526	1486.6478, 1492.3741, 1497.4772,
	C	-2.78917811	-0.49574427	-0.37600823	1503.5221, 1508.5367, 1512.4108,
	H	-2.64480915	-0.45184441	-1.45936062	1518.9661, 3033.5909, 3034.4483,
H	-2.23946204	-1.37174675	-0.02650667	3042.5774, 3049.3168, 3057.3876,	
C	-4.26891816	-0.66987150	-0.05891552	3058.9809, 3066.2531, 3068.9433,	
H	-4.84815926	0.17488781	-0.43422691	3082.6673, 3085.3645, 3093.6787,	
H	-4.42867734	-0.72615930	1.01890953	3103.1779, 3124.3639, 3132.2436,	
H	-4.67265079	-1.57821116	-0.50474435	3146.7348, 3792.8367	
O	5.02274230	-0.00226480	-0.31227735		
H	5.16590912	-0.79638769	-0.85057120		
SP1_33	C	-2.46706693	0.45666404	0.64530770	666.4499i, 32.5120, 46.9208, 67.4085,
	H	-2.25222528	1.51283960	0.80626305	83.9929, 94.8723, 133.7138, 150.7649,
	H	-3.50114532	0.43919358	0.11713534	199.7560, 279.6771, 294.6020,
	H	-2.59439794	-0.04464038	1.60456418	317.6842, 381.0321, 394.6719,
	C	-0.05790702	-0.23701701	0.36472995	505.6037, 719.9989, 730.8236,
	H	0.24376349	0.79338061	0.57242685	752.9875, 801.5041, 851.2151,
	H	-0.08554921	-0.75038065	1.33145465	866.6651, 937.3661, 965.4377,
	C	-1.45756987	-0.23014559	-0.24785750	970.5055, 1033.4845, 1042.6569,
	H	-1.77458257	-1.25751537	-0.43924797	1058.6260, 1077.4460, 1117.5081,
	H	-1.42361579	0.27073476	-1.21782707	1141.8317, 1174.4429, 1233.5433,
	C	0.97026162	-0.90887789	-0.53832668	1244.3867, 1260.6841, 1291.5657,
	H	1.04941902	-0.34449017	-1.47125851	1303.0313, 1325.9724, 1329.4002,
	H	0.60380628	-1.90035722	-0.81589115	1341.3839, 1368.1108, 1382.9137,
	C	2.35005285	-1.05426151	0.10201520	1389.9984, 1404.6533, 1415.0635,
	H	3.02509558	-1.52284053	-0.61903925	1455.3720, 1480.3671, 1488.1260,
	H	2.27658728	-1.74064536	0.94963314	1495.0558, 1498.4883, 1505.1078,
	C	2.97188321	0.25863850	0.57811892	1507.5051, 1517.9718, 1519.3458,
	H	2.38684541	0.66535651	1.40588823	3033.7049, 3042.5475, 3049.2848,
H	3.96263478	0.04692438	0.98418988	3056.8282, 3058.7047, 3059.3253,	
C	3.08989640	1.30355922	-0.52528903	3066.7097, 3077.8759, 3083.7099,	
H	2.10916218	1.63097527	-0.87217774	3088.0128, 3094.0345, 3102.1512,	
H	3.62597241	0.89931716	-1.38603525		

	H	3.62772851	2.18528454	-0.17902861	3123.3617, 3132.9672, 3147.7870,
	O	-4.80958894	0.22028217	-0.42638418	3790.2804
	H	-5.20008888	-0.17675266	0.36783229	
SP1_34	C	-2.48157049	0.21271237	0.76081506	667.3146i, 30.1074, 39.7518, 64.0907,
	H	-2.30236896	1.25773654	1.01270035	74.4433, 94.0435, 130.3579, 152.2377,
	H	-3.53158003	0.16102110	0.26729628	197.0048, 279.1964, 289.5661,
	H	-2.57281762	-0.37634348	1.67317320	317.5465, 380.1133, 393.6148,
	C	-0.05028731	-0.33736705	0.37170801	505.1323, 720.2189, 728.3036,
	H	0.20937666	0.68351912	0.66580494	756.1527, 805.9910, 850.4105,
	H	-0.03143398	-0.93593629	1.28821271	857.9416, 935.4207, 960.4869,
	C	-1.46302352	-0.34252646	-0.21006453	974.1890, 1031.3562, 1038.4329,
	H	-1.73647218	-1.36282428	-0.48669824	1060.6682, 1076.3757, 1117.2227,
	H	-1.47583302	0.24359026	-1.13178657	1142.7015, 1171.5485, 1233.2340,
	C	0.98541114	-0.87620965	-0.60861417	1248.0443, 1262.0715, 1289.1018,
	H	1.01711416	-0.22699355	-1.48768015	1302.3547, 1328.4770, 1332.4459,
	H	0.65731139	-1.85470062	-0.96804038	1338.8141, 1368.1665, 1383.8672,
	C	2.38497245	-1.01407062	-0.01105737	1388.2561, 1406.0029, 1414.2168,
	H	3.06317802	-1.38369718	-0.78472286	1455.6179, 1480.0028, 1487.8648,
	H	2.36201711	-1.77669154	0.77174442	1495.0263, 1497.6200, 1504.8611,
	C	2.95855247	0.27805238	0.57061838	1506.3563, 1517.3751, 1519.1457,
	H	2.37578044	0.58089378	1.44328612	3033.6090, 3042.5296, 3049.4381,
H	3.96705866	0.07703133	0.93637760	3056.3905, 3058.5796, 3059.0704,	
C	3.00393457	1.42274546	-0.43491881	3065.5780, 3077.9739, 3083.7842,	
H	2.00163335	1.73410259	-0.73142814	3087.8749, 3094.2680, 3101.3244,	
H	3.53689449	1.12323411	-1.33931547	3122.8293, 3131.9442, 3147.7720,	
H	3.51005805	2.29365513	-0.02017610	3791.7785	
O	-4.77518576	0.30531649	-0.43103924		
H	-4.87636633	1.25985253	-0.29135315		
SP1_35	C	-2.86813855	-0.58520714	0.45815674	772.7151i, 40.8662, 66.8248, 76.9724,
	H	-2.65729983	-0.67190943	1.52471621	90.8948, 121.8636, 137.3113,
	H	-2.89500861	0.55970017	0.24329303	173.6871, 246.0193, 256.9304,
	H	-3.89013101	-0.89504041	0.24915794	285.2850, 298.8338, 331.8329,
	C	-0.40079770	-1.11617860	0.05143737	422.9473, 533.9969, 662.2926,
	H	-0.29436451	-1.53794138	1.05611883	734.4024, 771.3755, 816.6206,
	H	0.24592422	-1.70382933	-0.60198368	863.6347, 874.5414, 908.6134,
	C	-1.84554575	-1.28785789	-0.41223281	949.3599, 975.5369, 1032.1527,
	H	-2.08194434	-2.35521122	-0.43129749	1046.6536, 1072.3341, 1090.2289,
	H	-1.94639758	-0.93929862	-1.44395901	1119.1182, 1136.7792, 1165.8136,
	C	0.07517791	0.33263440	0.07620662	1217.9389, 1254.1157, 1267.0723,
	H	-0.56480617	0.90877458	0.74883215	1288.9529, 1314.5061, 1325.7428,
	H	-0.04014627	0.76251501	-0.92711972	1335.3809, 1344.4028, 1350.8967,
	C	1.52621281	0.50033576	0.52200210	1392.7614, 1403.8351, 1408.9942,
	H	1.64638739	0.07100937	1.52167092	1414.1059, 1435.0779, 1480.2749,
	H	1.74760543	1.56634779	0.61951082	1486.5846, 1491.6048, 1497.9366,
	C	2.55165067	-0.12522435	-0.41773252	1504.1985, 1506.2969, 1510.9522,
	H	2.41170074	-1.20687009	-0.45658663	1513.8325, 3007.6942, 3036.4534,
H	2.38006631	0.24589822	-1.43218177	3040.6677, 3043.3873, 3050.4961,	
C	3.98182074	0.18151610	0.00811555	3057.2394, 3070.7881, 3073.6821,	
H	4.17387830	-0.19329584	1.01454483	3076.7624, 3087.9517, 3093.9745,	
H	4.16184243	1.25734355	0.01695626	3104.4230, 3124.8642, 3132.4838,	
H	4.70814599	-0.27504088	-0.66318662	3155.3521, 3786.0710	
O	-2.90307175	1.89298236	-0.26582899		
H	-2.00315925	1.86287985	-0.62757245		
SP1_36	C	-2.06382448	-0.01805602	0.62556054	671.7618i, 32.0017, 56.2164, 71.0595,
	H	-1.31854055	0.62921615	1.08665379	82.5392, 112.2101, 134.7548,
	H	-2.94957285	0.66566685	0.31711202	151.4252, 214.4722, 252.4851,
	H	-2.47814965	-0.69540087	1.37290617	264.0931, 342.2415, 379.7048,
	C	-0.50112921	-1.78799016	-0.30034589	

	H	-0.96055898	-2.58611106	0.28792274	403.3426, 502.9080, 716.5389,
	H	-0.17614478	-2.24079257	-1.24056372	726.7309, 750.6029, 818.9581,
	C	-1.56451552	-0.72967748	-0.61398789	854.4858, 866.0723, 918.0111,
	H	-2.40453435	-1.21237139	-1.11509837	948.8461, 978.3707, 1034.3451,
	H	-1.16557370	0.00219201	-1.31812821	1042.5239, 1072.1377, 1088.7213,
	C	0.72127878	-1.25732119	0.44649443	1114.1115, 1146.9167, 1164.5536,
	H	1.42791662	-2.07869115	0.58999391	1222.7195, 1249.9254, 1263.1624,
	H	0.43214506	-0.93105664	1.44960263	1294.2152, 1299.9085, 1326.1851,
	C	1.43236106	-0.11278495	-0.26536293	1333.3731, 1336.2904, 1366.6643,
	H	0.77229116	0.75786317	-0.32534119	1383.6703, 1388.0780, 1409.5670,
	H	1.64603185	-0.40417113	-1.29930475	1415.1093, 1453.6010, 1483.4715,
	C	2.72853266	0.29847647	0.42193644	1489.3810, 1494.3087, 1498.4975,
	H	2.51265344	0.56969893	1.45883231	1504.3414, 1504.9258, 1514.3319,
	H	3.39966873	-0.56306279	0.46467412	1523.3150, 3029.0502, 3043.6971,
	C	3.42307590	1.45794522	-0.27984600	3046.0089, 3050.3345, 3056.5825,
	H	2.77881780	2.33798397	-0.30534578	3057.1834, 3067.9699, 3076.1774,
	H	3.66546518	1.19700069	-1.31099811	3081.6703, 3086.4926, 3094.0051,
	H	4.34938212	1.73571552	0.22177700	3106.2806, 3122.6526, 3131.4529,
	O	-3.89097401	1.66172754	-0.10733125	3146.3628, 3790.6522
	H	-3.45818015	2.41894873	0.31726325	
	C	2.71592981	-0.67265973	-0.23532451	
	H	2.65673331	-0.84180604	-1.31115466	779.5986i, 42.9265, 62.5085, 90.2242,
	H	2.75586005	0.48523741	-0.10929657	111.4560, 136.9931, 159.2771,
	H	3.68456998	-0.99171991	0.14420655	194.3032, 235.6561, 282.6003,
	C	0.19717599	-1.10072386	-0.15330919	301.1978, 327.8499, 359.9324,
	H	0.21717719	-1.60396940	-1.12553646	443.1846, 521.0573, 660.5895,
	H	-0.55961635	-1.61370099	0.44383508	734.0654, 782.6609, 818.4733,
	C	1.55246183	-1.27228808	0.52868099	853.2937, 868.6507, 910.0637,
	H	1.74201253	-2.34019587	0.66688398	956.2650, 965.3790, 1012.5671,
	H	1.51733750	-0.84105382	1.53331686	1034.7365, 1069.8834, 1096.7333,
	C	-0.21466704	0.35259197	-0.35914191	1122.2209, 1136.0698, 1158.8666,
	H	0.53817894	0.86098908	-0.96601222	1199.7709, 1251.1017, 1260.6411,
	H	-0.23314952	0.85855841	0.61340574	1287.9769, 1306.1032, 1331.0664,
	C	-1.57108828	0.51639744	-1.04552809	1336.3660, 1341.5726, 1377.5290,
	H	-1.49958149	0.12325549	-2.06284395	1389.1975, 1393.2424, 1410.1867,
	H	-1.78792891	1.58345233	-1.14091848	1414.7744, 1434.5052, 1479.9527,
	C	-2.73984696	-0.16095413	-0.32973289	1484.6842, 1493.8651, 1497.6354,
	H	-3.65736153	0.06809286	-0.87449256	1504.0862, 1505.5373, 1509.5646,
	H	-2.62569641	-1.24589431	-0.37558501	1524.1451, 3021.0291, 3039.7507,
	C	-2.89107210	0.27573086	1.12276139	3041.9051, 3046.4071, 3055.9996,
	H	-2.94837975	1.36339129	1.19698359	3062.0506, 3072.2195, 3076.2843,
	H	-2.04590300	-0.05246993	1.72919290	3082.6659, 3087.3616, 3095.2209,
	H	-3.79470429	-0.13855278	1.56796600	3098.2575, 3122.5572, 3132.9240,
	O	2.74295010	1.85316454	0.29525880	3155.0145, 3786.4853
	H	1.80349152	1.87250299	0.53754415	
SP1_37	C	-2.02990354	0.58002286	0.08748181	
	H	-1.71753722	1.47121799	-0.45842445	683.0539i, 30.1077, 43.8062, 63.3798,
	H	-3.18847988	0.58225960	0.01505896	81.7084, 126.8279, 142.7352,
	H	-1.78509646	0.68774196	1.14273081	172.6918, 236.4592, 264.1277,
	C	0.00889552	-0.73033039	-0.65343066	294.3659, 324.3071, 357.7265,
	H	0.30855415	-1.65192637	-1.16062172	440.2989, 522.7705, 717.3674,
	H	0.32391762	0.09415325	-1.29934679	740.1956, 788.1542, 806.0053,
	C	-1.51633437	-0.70453750	-0.52912675	845.6041, 853.8968, 912.0802,
	H	-1.84655257	-1.55456307	0.07217027	946.4499, 965.9054, 1015.3650,
	H	-1.96038623	-0.82902337	-1.51770581	1035.7149, 1068.6724, 1085.9018,
	C	0.73173010	-0.64153877	0.68666385	1118.5134, 1144.0936, 1163.6541,
	H	0.30539511	-1.38208210	1.36944488	1205.2450, 1259.3013, 1262.0015,
	H	0.54607927	0.33372990	1.14239325	1294.9289, 1304.3282, 1324.1745,
SP1_38	C	-2.02990354	0.58002286	0.08748181	
	H	-1.71753722	1.47121799	-0.45842445	
	H	-3.18847988	0.58225960	0.01505896	
	H	-1.78509646	0.68774196	1.14273081	
	C	0.00889552	-0.73033039	-0.65343066	
	H	0.30855415	-1.65192637	-1.16062172	
	H	0.32391762	0.09415325	-1.29934679	
	C	-1.51633437	-0.70453750	-0.52912675	
	H	-1.84655257	-1.55456307	0.07217027	
	H	-1.96038623	-0.82902337	-1.51770581	
	C	0.73173010	-0.64153877	0.68666385	
	H	0.30539511	-1.38208210	1.36944488	
	H	0.54607927	0.33372990	1.14239325	

	C	2.23811546	-0.87401011	0.57945355	1341.3210, 1343.7725, 1373.9476,
	H	2.41658646	-1.90350117	0.25819077	1377.4266, 1388.3712, 1408.6575,
	H	2.68310478	-0.77636786	1.57320862	1414.1473, 1456.6350, 1480.1836,
	C	2.95627904	0.07737418	-0.37807050	1492.8396, 1496.1695, 1497.1169,
	H	4.02433152	-0.14601573	-0.35442104	1500.2809, 1506.7282, 1516.7199,
	H	2.62989930	-0.11447265	-1.40249640	1521.5921, 3037.2451, 3042.9986,
	C	2.73929746	1.54811942	-0.04097642	3049.9794, 3055.5326, 3056.9984,
	H	3.00621041	1.75146456	0.99785983	3060.8226, 3071.8672, 3079.7214,
	H	1.69699358	1.83996315	-0.17670076	3082.8789, 3092.3565, 3096.9199,
	H	3.34639262	2.19262932	-0.67549511	3102.6588, 3122.0622, 3131.1680,
	O	-4.61187838	0.43070788	0.11038832	3151.5949, 3792.5291
	H	-4.66286348	0.42853136	1.07907890	
	C	2.18018526	0.51920379	0.27897100	680.8901i, 39.9248, 41.9981, 50.4208,
	H	2.16282936	0.59574450	1.36659135	84.5087, 103.0446, 105.2283,
	H	3.28013039	0.68920813	-0.05164145	148.5726, 184.1819, 253.5879,
	H	1.63073761	1.35011183	-0.16012639	285.5368, 313.6129, 347.3882,
	C	0.34966803	-1.24063866	0.27062030	461.0289, 462.9096, 728.0667,
	H	0.13731033	-2.25899600	-0.06476323	742.3221, 766.1907, 779.1330,
	H	0.34531694	-1.26846453	1.36469870	835.9229, 892.8198, 928.7169,
	C	1.74446124	-0.84333641	-0.21877639	954.6364, 978.0294, 1013.4833,
	H	1.76088790	-0.85362379	-1.31074826	1035.6718, 1075.0688, 1096.7967,
	H	2.46718547	-1.59100537	0.11148846	1108.5100, 1141.1174, 1188.9107,
	C	-0.76284444	-0.31657966	-0.21133012	1214.2333, 1242.6729, 1267.2951,
	H	-0.72309192	-0.24136057	-1.30368483	1292.0915, 1308.0176, 1323.4737,
	H	-0.59327930	0.69054432	0.17471386	1331.6345, 1346.0683, 1375.5492,
	C	-2.14600008	-0.79912095	0.21126342	1381.4944, 1383.3028, 1410.1345,
	H	-2.20177952	-0.80893751	1.30461544	1414.7122, 1456.6400, 1483.4824,
	H	-2.27152587	-1.83579083	-0.11219403	1487.2161, 1492.9753, 1496.9862,
	C	-3.29418695	0.04095117	-0.34281433	1504.3893, 1507.2879, 1512.0984,
	H	-3.26285991	0.01298536	-1.43525156	1523.8536, 3028.4423, 3035.6495,
	H	-4.24061092	-0.41765809	-0.05040988	3043.9429, 3049.2945, 3058.5224,
	C	-3.27201370	1.49048812	0.12993401	3059.2048, 3070.8692, 3077.6891,
	H	-2.40113727	2.02334807	-0.25073659	3083.8137, 3087.6270, 3098.1106,
	H	-3.24263610	1.54050706	1.22008284	3104.2042, 3125.5051, 3135.6008,
	H	-4.15816225	2.02810771	-0.20549094	3152.5251, 3791.7439
	O	4.69819258	0.78290098	-0.24736847	
	H	4.92952826	0.97626751	0.67459691	
SP1_39	C	-2.37595555	-0.61056934	0.02580571	679.7768i, 28.0831, 43.4433, 52.3147,
	H	-2.43820650	-1.43797087	0.73339191	77.9976, 91.6183, 130.7312, 173.0741,
	H	-3.45086658	-0.17349054	-0.00695926	229.0277, 269.0249, 286.8280,
	H	-2.16812977	-0.99186009	-0.97221696	319.5743, 359.1735, 434.8011,
	C	-0.00760420	-0.01449132	0.73502512	517.6319, 719.4621, 731.4989,
	H	0.57385332	0.81135227	1.15090073	775.1483, 818.5172, 848.4742,
	H	-0.03101328	-0.79418667	1.50338500	854.2647, 910.7531, 945.7501,
	C	-1.43140704	0.48497897	0.47472016	967.3179, 1013.6437, 1035.7087,
	H	-1.40413472	1.27484191	-0.27970145	1065.8172, 1086.2628, 1119.8479,
	H	-1.82311427	0.93899370	1.38600355	1137.6808, 1173.6536, 1203.8381,
	C	0.69065677	-0.55336814	-0.50857467	1258.0700, 1266.4025, 1295.5772,
	H	0.72381012	0.23362063	-1.26780514	1302.6357, 1327.5784, 1338.6586,
	H	0.09975547	-1.36479690	-0.93803084	1346.0101, 1375.5242, 1378.6128,
	C	2.10131238	-1.07800877	-0.24055662	1389.1045, 1409.9733, 1414.5985,
	H	2.53024080	-1.42674318	-1.18372695	1458.2393, 1480.3800, 1490.9603,
	H	2.03536754	-1.95275943	0.41173283	1495.5608, 1496.0840, 1500.1859,
	C	3.05584608	-0.06149485	0.38638022	1506.5503, 1516.4914, 1524.1641,
	H	2.73148300	0.17513180	1.40184234	3034.1794, 3042.8841, 3047.9916,
	H	4.03906490	-0.52502456	0.48488210	3056.1651, 3056.4182, 3061.0609,
	C	3.18109939	1.22454468	-0.42211587	3076.7968, 3080.6929, 3084.9375,
	H	2.24316206	1.78095857	-0.43530167	
SP1_40	C	-2.37595555	-0.61056934	0.02580571	679.7768i, 28.0831, 43.4433, 52.3147,
	H	-2.43820650	-1.43797087	0.73339191	77.9976, 91.6183, 130.7312, 173.0741,
	H	-3.45086658	-0.17349054	-0.00695926	229.0277, 269.0249, 286.8280,
	H	-2.16812977	-0.99186009	-0.97221696	319.5743, 359.1735, 434.8011,
	C	-0.00760420	-0.01449132	0.73502512	517.6319, 719.4621, 731.4989,
	H	0.57385332	0.81135227	1.15090073	775.1483, 818.5172, 848.4742,
	H	-0.03101328	-0.79418667	1.50338500	854.2647, 910.7531, 945.7501,
	C	-1.43140704	0.48497897	0.47472016	967.3179, 1013.6437, 1035.7087,
	H	-1.40413472	1.27484191	-0.27970145	1065.8172, 1086.2628, 1119.8479,
	H	-1.82311427	0.93899370	1.38600355	1137.6808, 1173.6536, 1203.8381,
	C	0.69065677	-0.55336814	-0.50857467	1258.0700, 1266.4025, 1295.5772,
	H	0.72381012	0.23362063	-1.26780514	1302.6357, 1327.5784, 1338.6586,
	H	0.09975547	-1.36479690	-0.93803084	1346.0101, 1375.5242, 1378.6128,
	C	2.10131238	-1.07800877	-0.24055662	1389.1045, 1409.9733, 1414.5985,
	H	2.53024080	-1.42674318	-1.18372695	1458.2393, 1480.3800, 1490.9603,
	H	2.03536754	-1.95275943	0.41173283	1495.5608, 1496.0840, 1500.1859,
	C	3.05584608	-0.06149485	0.38638022	1506.5503, 1516.4914, 1524.1641,
	H	2.73148300	0.17513180	1.40184234	3034.1794, 3042.8841, 3047.9916,
	H	4.03906490	-0.52502456	0.48488210	3056.1651, 3056.4182, 3061.0609,
	C	3.18109939	1.22454468	-0.42211587	3076.7968, 3080.6929, 3084.9375,
	H	2.24316206	1.78095857	-0.43530167	

	H	3.44996272	1.00681755	-1.45754690	3094.5695, 3097.0129, 3101.1273,
	H	3.94637351	1.87947375	-0.00742224	3122.4284, 3132.5167, 3153.1642,
	O	-4.70476192	0.48008589	-0.25146217	3792.0208
	H	-4.70319991	0.37540765	-1.21583411	
SP1_41	C	2.04727219	-0.15166702	0.58867885	682.7747i, 30.4705, 36.7462, 42.9987,
	H	1.38718477	-0.98649194	0.82220010	79.6192, 82.8986, 123.5578, 192.3575,
	H	3.02749640	-0.65038250	0.21588648	231.6357, 243.8163, 293.8163,
	H	2.29524380	0.38928120	1.50248049	321.1207, 363.3167, 434.4663,
	C	0.30368040	1.56594687	-0.07517291	514.0256, 717.3380, 745.6379,
	H	0.60760258	2.27180201	0.70195650	749.7650, 796.5992, 855.8776,
	H	-0.03299881	2.16503087	-0.92514709	868.5679, 909.4248, 957.2378,
	C	1.52892136	0.75342095	-0.50856929	975.2400, 1003.8951, 1038.7749,
	H	2.31906285	1.44246291	-0.81032644	1069.0942, 1092.2652, 1116.3862,
	H	1.28965639	0.15683474	-1.38988872	1140.8552, 1165.7806, 1212.4206,
	C	-0.86811397	0.73262355	0.44282018	1243.6374, 1262.6648, 1295.3478,
	H	-1.68126833	1.41289183	0.70172948	1297.3268, 1328.9820, 1335.8687,
	H	-0.58538110	0.22938572	1.37257808	1348.7517, 1378.4158, 1379.5985,
	C	-1.36813967	-0.30861061	-0.55296545	1388.6671, 1409.4392, 1416.2669,
	H	-0.55823761	-1.00288386	-0.78882542	1456.5974, 1483.0102, 1490.2808,
	H	-1.62951398	0.19002614	-1.49261443	1492.7263, 1499.2601, 1504.5199,
	C	-2.56937268	-1.11001374	-0.05507063	1507.3231, 1513.0344, 1523.1495,
	H	-2.78836026	-1.90037570	-0.77533005	3031.5073, 3045.5226, 3046.2318,
H	-2.30144436	-1.61144436	0.87899354	3049.2839, 3059.4657, 3068.6423,	
C	-3.82343259	-0.26924149	0.15857127	3077.1105, 3081.0732, 3085.6332,	
H	-4.07764961	0.28099543	-0.74924326	3086.7619, 3100.5805, 3108.1291,	
H	-3.69214283	0.45587913	0.96094128	3125.8076, 3137.0318, 3145.4920,	
H	-4.67621900	-0.89509076	0.41929955	3792.2256	
O	4.34827714	-1.06480317	-0.15666979		
H	4.80586181	-0.70424658	0.61891607		
SP1_42	C	-2.07435852	0.01260609	-0.65819809	669.7801i, 30.6686, 33.6794, 63.2008,
	H	-1.43312818	-0.83013372	-0.91440445	85.8704, 113.4960, 124.6590,
	H	-3.09508372	-0.43504239	-0.33470505	187.2448, 222.3372, 244.4751,
	H	-2.29262016	0.59662545	-1.55278408	294.1969, 336.0113, 358.8263,
	C	-0.28126033	1.63226999	0.11185572	434.8434, 514.6833, 715.9009,
	H	-0.54302578	2.38149432	-0.63937656	726.1585, 757.3308, 811.0858,
	H	0.06000254	2.18133350	0.99321934	850.2457, 869.6738, 903.1750,
	C	-1.54462791	0.84944471	0.48687561	958.8849, 963.7681, 1025.9331,
	H	-2.31354475	1.55558912	0.80301652	1036.6578, 1071.2173, 1093.1002,
	H	-1.34659002	0.20693933	1.34602090	1115.9912, 1146.5783, 1155.1414,
	C	0.86892918	0.77792667	-0.41999085	1215.8232, 1247.1027, 1263.9227,
	H	1.71167615	1.43720024	-0.63476447	1293.0042, 1304.4005, 1327.2456,
	H	0.58635919	0.32571239	-1.37563575	1333.5243, 1346.5562, 1376.2170,
	C	1.31085133	-0.32233527	0.53901681	1378.4678, 1388.9379, 1408.6030,
	H	0.47051408	-0.99322425	0.73279542	1416.5338, 1454.1831, 1482.6712,
	H	1.57415613	0.12624534	1.50299475	1489.8632, 1492.8017, 1498.4874,
	C	2.48912653	-1.14893648	0.02755554	1504.4413, 1507.4892, 1512.3872,
	H	2.66420783	-1.97723148	0.71663042	1523.4780, 3031.9731, 3045.9673,
H	2.21958679	-1.59910257	-0.93187793	3046.4214, 3048.8722, 3059.3339,	
C	3.77843346	-0.34986112	-0.12849217	3068.1724, 3076.7063, 3081.9703,	
H	4.03711672	0.15026103	0.80660878	3086.0637, 3086.7139, 3100.2499,	
H	3.68958581	0.41385886	-0.90027213	3107.4234, 3126.0355, 3136.1489,	
H	4.61100047	-0.99693026	-0.40239888	3146.3568, 3791.7587	
O	-4.24189643	-1.15184878	0.14493258		
H	-3.94760414	-2.03549220	-0.12626286		
SP2_1	C	-3.37625914	-1.14795850	-0.12898840	489.1324i, 47.2193, 50.1656, 72.6715,
	H	-3.29671618	-2.18941588	0.19094136	102.2640, 108.6920, 118.9088,
	H	-4.31758083	-0.75014480	0.24635194	144.5657, 153.7395, 236.7526,
	H	-3.41222924	-1.13615610	-1.21844020	

	C	-0.84750751	-0.81262043	-0.15074733	248.6810, 251.1929, 307.0455,
	H	-0.68974691	-1.85386075	0.15332433	419.1425, 487.6389, 627.8588,
	H	-0.87196643	-0.81205015	-1.24426126	729.3027, 750.4838, 810.0252,
	C	-2.19125974	-0.34995323	0.37660755	864.8304, 900.7043, 930.9404,
	H	-2.33838161	0.73067172	0.02253981	940.1904, 1021.7187, 1024.8791,
	H	-2.18307942	-0.29557231	1.46789756	1068.6647, 1087.1438, 1093.8982,
	C	0.31723298	0.04069773	0.33287745	1099.2473, 1168.5627, 1201.9200,
	H	0.33007582	0.04900091	1.42769283	1238.2995, 1244.6806, 1256.8337,
	H	0.15426720	1.07429526	0.01337311	1300.7887, 1313.7171, 1328.9546,
	C	1.66724741	-0.44043195	-0.18185900	1335.2451, 1343.6650, 1365.8160,
	H	1.65304955	-0.45242259	-1.27612052	1399.6924, 1407.5206, 1411.5127,
	H	1.82886416	-1.47621104	0.13325619	1415.0240, 1479.2837, 1487.6938,
	C	2.83220462	0.41729586	0.29540224	1493.1731, 1494.4905, 1499.8411,
	H	2.66903393	1.45032266	-0.02212027	1503.8122, 1505.1597, 1514.3834,
	H	2.84347167	0.43005879	1.38843677	1666.2445, 3024.2443, 3030.2441,
	C	4.17514430	-0.07575977	-0.22707194	3037.1606, 3049.3985, 3053.4734,
	H	4.19136320	-0.07095966	-1.31784290	3056.6164, 3057.7286, 3061.6574,
	H	4.36667588	-1.09836611	0.10123014	3072.4301, 3082.8006, 3093.4973,
	H	4.99711297	0.54777529	0.12280998	3118.8183, 3124.2580, 3131.3076,
	O	-2.41330274	2.19363648	-0.32648999	3141.9261, 3780.9728
	H	-2.07860925	2.51632470	0.52552766	
	C	-3.04163306	-0.49414199	0.30766752	642.8225i, 35.6119, 50.7239, 77.9223,
	H	-3.79650457	0.29454126	0.33973234	118.7504, 131.4301, 184.8517,
	H	-3.45192142	-1.33794266	-0.24429911	202.4416, 209.6521, 239.9070,
	H	-2.85237732	-0.82032944	1.33075229	260.1075, 294.8020, 316.8679,
	C	-1.08909484	1.12976052	0.44384104	432.4026, 516.0888, 661.2373,
	H	-1.83793657	1.90271014	0.64501160	727.9137, 749.7035, 791.2684,
	H	-0.78394423	0.75297761	1.42366732	846.7196, 877.2396, 893.9137,
	C	-1.76653895	0.01533919	-0.33152310	947.7910, 972.9846, 1049.8018,
	H	-1.07094001	-0.90001432	-0.40244320	1055.6522, 1057.8385, 1071.2247,
	H	-1.92195978	0.30060154	-1.37544526	1114.8692, 1156.8216, 1166.5631,
	C	0.09262570	1.77371464	-0.28014548	1182.0702, 1249.0700, 1259.0207,
	H	0.49091357	2.58186201	0.33874157	1301.0995, 1311.0046, 1329.2394,
	H	-0.27450182	2.23924047	-1.19822031	1342.8319, 1359.6983, 1390.6129,
	C	1.22638336	0.81307677	-0.63240853	1398.4497, 1407.2863, 1409.7945,
	H	1.98929427	1.35559539	-1.19639421	1419.0759, 1483.8622, 1491.8573,
	H	0.85635002	0.03326394	-1.30493629	1492.8270, 1497.6055, 1499.4375,
	C	1.88945360	0.16965195	0.58148425	1500.8557, 1504.9214, 1521.6644,
	H	2.28265069	0.95550051	1.23162455	1623.6115, 3034.8348, 3040.2151,
	H	1.14494647	-0.36039979	1.18287886	3047.9597, 3048.3806, 3051.2953,
	C	3.01254255	-0.78387175	0.19001909	3053.9556, 3062.4480, 3066.5419,
	H	3.78969262	-0.25541717	-0.36325634	3074.3420, 3088.3104, 3092.1562,
	H	2.64697368	-1.58297764	-0.45969123	3113.4557, 3119.2206, 3134.5648,
	H	3.47393111	-1.24594242	1.06168748	3142.7003, 3779.4803
	O	-0.38781948	-2.22260593	-0.32874681	
	H	0.47545908	-1.87359801	-0.05304431	
SP2_2	C	-3.04190060	-0.49184919	0.30145208	642.5716i, 18.1660, 47.6680, 78.8855,
	H	-3.79645664	0.29731258	0.32847714	117.6927, 129.8485, 184.7253,
	H	-3.44985742	-1.33625551	-0.25134151	201.1225, 208.7145, 239.6924,
	H	-2.85780593	-0.81656225	1.32593454	259.5284, 294.8174, 316.5225,
	C	-1.08848716	1.13036653	0.44541928	432.1256, 516.3715, 667.8448,
	H	-1.83834502	1.90245955	0.64607820	725.2757, 747.4861, 791.4484,
	H	-0.78436382	0.75270896	1.42518886	846.8642, 877.7783, 893.6155,
	C	-1.76327952	0.01586319	-0.33208586	947.6568, 972.8112, 1048.8868,
	H	-1.06881717	-0.90072216	-0.39557782	1055.5009, 1057.5846, 1070.9005,
	H	-1.91314035	0.29946252	-1.37724461	1114.6213, 1156.7682, 1165.9336,
	C	0.09372308	1.77615509	-0.27604910	1181.4928, 1248.5931, 1258.2739,
	H	0.49237346	2.58187840	0.34572878	
SP2_3	C	-3.04190060	-0.49184919	0.30145208	642.5716i, 18.1660, 47.6680, 78.8855,
	H	-3.79645664	0.29731258	0.32847714	117.6927, 129.8485, 184.7253,
	H	-3.44985742	-1.33625551	-0.25134151	201.1225, 208.7145, 239.6924,
	H	-2.85780593	-0.81656225	1.32593454	259.5284, 294.8174, 316.5225,
	C	-1.08848716	1.13036653	0.44541928	432.1256, 516.3715, 667.8448,
	H	-1.83834502	1.90245955	0.64607820	725.2757, 747.4861, 791.4484,
	H	-0.78436382	0.75270896	1.42518886	846.8642, 877.7783, 893.6155,
	C	-1.76327952	0.01586319	-0.33208586	947.6568, 972.8112, 1048.8868,
	H	-1.06881717	-0.90072216	-0.39557782	1055.5009, 1057.5846, 1070.9005,
	H	-1.91314035	0.29946252	-1.37724461	1114.6213, 1156.7682, 1165.9336,
	C	0.09372308	1.77615509	-0.27604910	1181.4928, 1248.5931, 1258.2739,
	H	0.49237346	2.58187840	0.34572878	

	H	-0.27264766	2.24503227	-1.19272346	1301.4245, 1311.0192, 1329.3114,
	C	1.22720825	0.81623141	-0.63100049	1343.2287, 1358.4443, 1390.5268,
	H	1.99234352	1.36120461	-1.18960494	1398.3151, 1407.2684, 1409.7063,
	H	0.85764361	0.04194982	-1.31046496	1419.2911, 1483.7187, 1491.7433,
	C	1.88539045	0.16381711	0.58075104	1492.6957, 1497.3871, 1499.1381,
	H	2.27270537	0.94520900	1.23970989	1500.7563, 1504.9000, 1521.3873,
	H	1.13924771	-0.37467437	1.17212154	1628.3520, 3034.9579, 3040.3828,
	C	3.01404078	-0.78229320	0.18726767	3047.1346, 3048.1054, 3051.6058,
	H	3.79302857	-0.24655871	-0.35635463	3054.0195, 3062.6770, 3067.0207,
	H	2.65594420	-1.57709196	-0.47201429	3074.4611, 3088.3426, 3091.8954,
	H	3.47118947	-1.25124315	1.05745261	3112.8296, 3119.3798, 3134.8874,
	O	-0.39290610	-2.22707271	-0.31696450	3142.6786, 3778.5550
	H	0.49003515	-1.87727350	-0.11417708	
SP2_4	C	-3.36171802	-1.14281161	-0.14052316	494.8843i, 38.1789, 41.1124, 67.4108,
	H	-3.28526600	-2.19718048	0.13454320	86.8092, 98.4053, 103.3912, 141.7284,
	H	-4.30046604	-0.75733271	0.25364194	147.4779, 231.6602, 248.2924,
	H	-3.40043655	-1.08385545	-1.22835310	250.4655, 307.6908, 418.8859,
	C	-0.83152507	-0.81349887	-0.15425218	487.8131, 625.5947, 729.0295,
	H	-0.66971203	-1.86390756	0.11387846	750.0104, 805.8751, 858.9531,
	H	-0.86162589	-0.77593297	-1.24699167	900.0253, 929.8836, 939.9712,
	C	-2.17336353	-0.37032574	0.39447367	1022.3850, 1025.2568, 1068.9074,
	H	-2.31448393	0.72173422	0.08140531	1087.0511, 1093.7653, 1099.0018,
	H	-2.16270761	-0.35795564	1.48704119	1168.9980, 1201.2013, 1227.3463,
	C	0.33255022	0.02740350	0.35208639	1247.2050, 1257.6110, 1300.5843,
	H	0.35436679	-0.00544656	1.44621811	1313.3609, 1332.0191, 1335.0159,
	H	0.16072510	1.07168565	0.07411743	1365.0211, 1381.7835, 1399.1335,
	C	1.68096557	-0.42535295	-0.19160909	1407.7515, 1411.3117, 1414.7028,
	H	1.65794331	-0.39514101	-1.28537100	1478.8091, 1487.4928, 1492.7813,
	H	1.85095146	-1.47160681	0.08176565	1494.4386, 1499.1327, 1503.9267,
	C	2.84497280	0.42005262	0.30932717	1504.5580, 1514.1717, 1659.3743,
	H	2.67303243	1.46375811	0.03416203	3024.4973, 3029.9640, 3037.0608,
	H	2.86550413	0.39001183	1.40188600	3049.1819, 3053.9995, 3055.7503,
	C	4.18624776	-0.04371645	-0.24336942	3057.2661, 3061.5675, 3072.4395,
H	4.19314942	0.00442004	-1.33319147	3082.6532, 3092.9461, 3119.1869,	
H	4.38646833	-1.07739103	0.04233336	3123.8396, 3130.9381, 3141.8954,	
H	5.00760528	0.57042262	0.12414867	3782.0530	
O	-2.50107873	2.16377349	-0.33162483		
H	-2.21519666	2.54302688	0.51496423		
SP2_5	C	-3.35246974	-1.06295978	-0.17968517	647.4827i, 42.4935, 52.7274, 77.1557,
	H	-3.28653736	-2.14915551	-0.08984862	100.9798, 107.7924, 115.2903,
	H	-4.28234315	-0.74620282	0.29181479	143.6836, 150.5477, 236.4462,
	H	-3.40703890	-0.82711579	-1.24400671	247.3188, 251.3485, 307.9710,
	C	-0.82341921	-0.75314822	-0.19656063	420.7401, 487.4772, 624.2957,
	H	-0.66811989	-1.83606960	-0.12730252	724.6993, 735.5269, 775.9416,
	H	-0.87986951	-0.51675928	-1.26341953	851.7310, 897.3544, 928.7245,
	C	-2.14547779	-0.40294185	0.45558019	945.9537, 1020.3713, 1024.3515,
	H	-2.25573043	0.73693087	0.36766191	1068.6716, 1086.4635, 1095.6731,
	H	-2.11403484	-0.57630507	1.53395050	1108.1939, 1163.3482, 1182.7453,
	C	0.36066862	-0.02321625	0.42302205	1230.2099, 1255.4307, 1271.8394,
	H	0.41636463	-0.26384792	1.48925541	1299.1335, 1313.3948, 1334.0454,
	H	0.18489919	1.05414730	0.35673217	1336.3963, 1365.8991, 1390.1681,
	C	1.68723951	-0.36562036	-0.24130280	1405.4192, 1410.2528, 1411.3393,
	H	1.63124954	-0.12234286	-1.30699778	1416.0054, 1477.2565, 1487.1062,
	H	1.85681037	-1.44566252	-0.18270790	1493.2620, 1497.9696, 1500.2982,
	C	2.87345983	0.36293067	0.37738630	1503.2157, 1504.5729, 1514.1845,
	H	2.70118270	1.44046697	0.31805885	1690.0396, 3024.2296, 3030.2463,
	H	2.92795876	0.11922014	1.44155338	3040.5302, 3050.4445, 3051.1311,
	C	4.19269731	0.01372611	-0.29879209	

	H	4.16568556	0.27436525	-1.35780894	3056.9626, 3057.8423, 3060.4934,
	H	4.39347125	-1.05628811	-0.22749464	3075.2559, 3083.2608, 3094.9901,
	H	5.03035210	0.54244908	0.15472615	3113.2652, 3123.8649, 3130.0312,
	O	-2.48483051	2.11073534	-0.18976621	3131.4857, 3782.9510
	H	-3.29184710	1.87366518	-0.67392400	
SP2_6	C	2.60158698	-0.59257656	0.45002713	543.8716i, 60.4224, 79.3249, 91.3585,
	H	2.95145284	-1.61618634	0.29491780	100.6462, 111.0434, 145.1784,
	H	3.47332883	0.05964552	0.48300335	198.3799, 207.5724, 256.7494,
	H	2.11665535	-0.54933809	1.42469691	326.6177, 341.3815, 387.9558,
	C	0.45444162	-1.10813059	-0.85311071	439.6293, 517.2498, 642.1324,
	H	-0.18679093	-0.70205577	-1.63835283	729.9524, 771.8305, 800.9219,
	H	0.83077888	-2.06489481	-1.23051884	834.7977, 873.5330, 887.7254,
	C	1.64903660	-0.18489281	-0.65744506	950.9033, 964.7361, 1004.7149,
	H	1.24871650	0.86295139	-0.39877059	1050.7852, 1051.4781, 1073.5867,
	H	2.17840000	-0.04956367	-1.60194902	1103.5979, 1157.9968, 1163.7098,
	C	-0.36750589	-1.36365959	0.40924716	1180.5625, 1223.0919, 1250.8447,
	H	0.24387666	-1.89779552	1.13973837	1288.7111, 1316.4649, 1338.2623,
	H	-1.18798061	-2.03873586	0.15779729	1353.6753, 1362.1195, 1378.7088,
	C	-0.92465230	-0.09497699	1.05683353	1395.2725, 1400.7652, 1412.3112,
	H	-0.10316791	0.51685679	1.43636399	1416.1544, 1475.5700, 1487.4977,
	H	-1.52340348	-0.38487047	1.92451731	1492.1901, 1497.2082, 1499.2181,
	C	-1.78314228	0.76152681	0.12664298	1506.0752, 1509.5671, 1519.1868,
	H	-2.14005539	1.62687439	0.68752060	1727.3909, 3034.1410, 3047.7361,
H	-1.16518806	1.16685084	-0.67678712	3052.9656, 3053.2749, 3062.4992,	
C	-2.97241205	0.00952948	-0.46024213	3068.5341, 3080.0475, 3085.4104,	
H	-3.57326379	-0.44603290	0.32952182	3089.1944, 3097.7468, 3102.1931,	
H	-2.65186032	-0.78861324	-1.13112850	3120.0249, 3121.4206, 3129.4526,	
H	-3.61880970	0.67618132	-1.03010711	3140.1462, 3786.1955	
O	1.14441679	2.31132564	-0.02756667		
H	2.00786077	2.57720291	-0.38164743		
SP2_7	C	2.19572720	-0.33417716	1.40095333	563.7606i, 45.7354, 74.6826, 83.4509,
	H	2.60678337	-1.33691465	1.54488738	94.8240, 129.2199, 166.9059,
	H	2.82912920	0.37163255	1.93493769	188.1631, 202.1102, 254.9235,
	H	1.20834695	-0.31298431	1.86223026	266.6606, 288.8804, 374.4604,
	C	1.34323031	-0.97828593	-0.93390318	401.8259, 508.3232, 662.1114,
	H	1.25008848	-0.57022357	-1.94378490	752.4730, 770.4571, 802.2883,
	H	1.93579455	-1.89389264	-1.02765378	846.0073, 857.4193, 920.8335,
	C	2.12996789	0.00200747	-0.07569352	950.5060, 979.5387, 1029.9923,
	H	1.68295686	1.05817823	-0.17259958	1043.2082, 1072.7594, 1095.9137,
	H	3.12922766	0.13998648	-0.49085269	1126.3483, 1160.9858, 1172.7625,
	C	-0.04152880	-1.34663259	-0.40558045	1206.8937, 1243.2528, 1264.0358,
	H	0.05301840	-1.86208951	0.55389763	1272.4876, 1300.8481, 1322.0579,
	H	-0.49678322	-2.06583915	-1.09085491	1333.6589, 1359.6093, 1379.6004,
	C	-0.98251285	-0.15956141	-0.24080185	1385.1068, 1406.6787, 1411.3031,
	H	-1.03964200	0.38830934	-1.18997032	1415.6157, 1476.8929, 1488.8344,
	H	-0.57874872	0.53380027	0.50365383	1491.8436, 1493.7197, 1504.4833,
	C	-2.38915079	-0.56657270	0.18043691	1505.3976, 1509.2726, 1521.2037,
	H	-2.80075493	-1.25470045	-0.56204504	1616.7039, 3009.1053, 3035.9836,
H	-2.33054404	-1.12529622	1.11802925	3047.2382, 3049.5765, 3052.5721,	
C	-3.31803518	0.62839029	0.34937037	3056.5434, 3058.8695, 3073.5519,	
H	-3.40939365	1.18354752	-0.58551928	3082.8466, 3091.0917, 3094.5919,	
H	-2.93364538	1.31445953	1.10540898	3116.9744, 3122.4339, 3134.1479,	
H	-4.31778740	0.32102330	0.65351812	3143.7667, 3782.4037	
O	1.16161977	2.43650872	-0.39328821		
H	0.29280901	2.14792567	-0.71566670		
SP2_8	C	-2.93984693	-1.44920082	-0.38938336	493.7002i, 27.5909, 61.5541, 76.7490,
	H	-2.75985183	-2.45092168	0.00760819	93.3922, 101.3124, 121.1404,
	H	-3.99777222	-1.22282548	-0.26806370	

	H	-2.71600312	-1.46862459	-1.45606823	136.7298, 205.2070, 239.3158,
	C	-0.57652996	-0.65909450	0.15802833	242.6844, 271.7612, 312.0579,
	H	-0.31614798	-1.63533783	0.58495165	402.4046, 518.2115, 629.8155,
	H	-0.34533647	-0.71600194	-0.90807926	734.2083, 757.6405, 817.8993,
	C	-2.06690272	-0.43617772	0.32355704	860.8005, 875.4117, 925.2079,
	H	-2.30927950	0.59063827	-0.12707879	943.9479, 988.7885, 1032.1031,
	H	-2.33322471	-0.35311539	1.37993790	1058.5123, 1080.6141, 1096.8151,
	C	0.26522887	0.42567621	0.82089623	1110.4556, 1164.2011, 1190.1324,
	H	-0.07639851	0.55562053	1.85192317	1240.9585, 1248.7044, 1270.6597,
	H	0.08112419	1.37365398	0.30650005	1295.8772, 1310.1320, 1330.5771,
	C	1.76314354	0.13418323	0.82425546	1331.8482, 1344.3528, 1370.3986,
	H	1.95266788	-0.78751909	1.38373707	1404.7584, 1406.0687, 1409.0315,
	H	2.28143142	0.93157508	1.36351572	1413.2849, 1479.1872, 1487.2260,
	C	2.37476306	0.00646815	-0.56700421	1493.9153, 1497.5374, 1498.9243,
	H	1.93890091	-0.85011839	-1.08475286	1501.0575, 1503.4893, 1512.5950,
	H	2.11168365	0.88964343	-1.15580309	1663.6525, 3019.9318, 3032.9627,
	C	3.88904144	-0.15086622	-0.51771857	3038.1347, 3050.3821, 3053.3333,
	H	4.16722737	-1.03484870	0.05820345	3056.6885, 3065.7318, 3067.5763,
	H	4.35359189	0.71316627	-0.04052991	3073.3923, 3092.1522, 3096.1919,
	H	4.31588717	-0.25330469	-1.51475412	3118.4794, 3123.2458, 3132.4831,
	O	-2.53230293	2.00966323	-0.57316607	3142.6581, 3782.1999
	H	-2.34346053	2.41508436	0.28829589	
	C	-2.79419721	-1.67194202	-0.18955800	
	H	-2.38570562	-2.63093677	0.13702561	485.8051i, 31.7160, 56.7241, 68.6120,
	H	-3.82882074	-1.61416831	0.14443549	96.2833, 110.8540, 129.5495,
	H	-2.78795334	-1.66094974	-1.27961485	132.7628, 205.0303, 232.2437,
	C	-0.52448896	-0.50860825	-0.11205060	247.0648, 275.4139, 312.6563,
	H	-0.05167374	-1.45135959	0.18143472	402.9698, 517.1360, 622.6566,
	H	-0.50655651	-0.48034823	-1.20606280	731.8492, 759.7984, 834.8292,
	C	-1.96449223	-0.53013355	0.36220818	855.7770, 874.6447, 922.9916,
	H	-2.44957700	0.44418916	0.00295009	940.6843, 989.5298, 1037.7992,
	H	-2.01393455	-0.49158505	1.45323283	1058.0932, 1080.7538, 1092.4687,
	C	0.26587003	0.67161773	0.44130936	1110.3955, 1161.9007, 1193.4866,
	H	0.31109788	0.59171600	1.53236121	1231.8695, 1245.6617, 1273.8365,
	H	-0.28374538	1.58866398	0.21500622	1293.5840, 1310.5621, 1330.3684,
	C	1.68242471	0.78480736	-0.11446885	1341.6191, 1346.6417, 1370.3817,
	H	2.14956993	1.69079719	0.28070672	1401.8256, 1407.1809, 1409.7131,
	H	1.63476706	0.91390397	-1.20028434	1412.8353, 1478.5954, 1486.8967,
	C	2.57793399	-0.40703655	0.20690687	1493.5832, 1496.6863, 1498.7909,
	H	2.56035761	-0.58747708	1.28567261	1500.8283, 1504.2355, 1512.1292,
	H	2.17818784	-1.30763583	-0.26326303	1667.7920, 3030.4383, 3035.1711,
	C	4.01271131	-0.19118712	-0.25709905	3038.5851, 3047.4690, 3053.9535,
	H	4.45046690	0.68180270	0.22900416	3056.4137, 3059.9084, 3069.4732,
	H	4.04833772	-0.02099455	-1.33417467	3073.4478, 3090.3548, 3092.4091,
	H	4.64274277	-1.05134813	-0.03333729	3119.1374, 3123.3734, 3131.1937,
	O	-3.02686542	1.79362974	-0.34109281	3141.6236, 3784.3282
	H	-2.98720727	2.15158669	0.56016222	
	C	-3.32603258	-0.99556508	0.20415466	
	H	-3.27202729	-2.01946726	0.58099596	489.6793i, 31.6740, 56.6663, 72.3463,
	H	-4.16762421	-0.50179950	0.68698701	86.1667, 97.9002, 124.4762, 142.7762,
	H	-3.52873785	-1.04476145	-0.86580541	147.8580, 234.0984, 243.6832,
	C	-0.81390040	-0.86670260	-0.21911323	287.8129, 356.8338, 396.6211,
	H	-0.68282853	-1.89669342	0.13261170	494.5242, 626.2990, 733.1875,
	H	-1.00846657	-0.93135807	-1.29345557	764.6776, 806.1306, 859.3944,
	C	-2.02373476	-0.26742080	0.46992598	889.0809, 924.8947, 945.8151,
	H	-2.14773039	0.79910993	0.06758441	984.9387, 1026.9202, 1059.1954,
	H	-1.84348480	-0.15042664	1.54122585	1083.8023, 1096.3660, 1108.5766,
	C	0.46916568	-0.08178799	0.02042795	1161.9577, 1192.3845, 1236.0643,
SP2_9					
SP2_10					

	H	0.63681808	0.00355467	1.09757648	1241.7181, 1260.2228, 1300.6820,
	H	0.33851411	0.93605547	-0.36091154	1312.5081, 1329.3979, 1343.2431,
	C	1.68336062	-0.71884893	-0.64588636	1345.5215, 1379.4870, 1390.6015,
	H	1.45591815	-0.88659815	-1.70179315	1405.9402, 1410.4773, 1415.7931,
	H	1.85646744	-1.70665049	-0.20680413	1479.1967, 1484.6273, 1492.5529,
	C	2.95952760	0.11154458	-0.53454650	1493.3991, 1499.4038, 1505.3540,
	H	3.75397945	-0.38382000	-1.09575177	1506.9047, 1512.2120, 1666.6601,
	H	2.79886717	1.07943897	-1.01655069	3024.3260, 3033.0575, 3043.1243,
	C	3.42062495	0.32825160	0.90263819	3049.7784, 3054.1606, 3058.1512,
	H	3.53159459	-0.62630552	1.42062446	3060.1480, 3068.5465, 3078.0539,
	H	2.70805290	0.93042982	1.46574198	3086.6743, 3095.7234, 3119.2108,
	H	4.38163015	0.84030234	0.93576675	3125.4839, 3135.0830, 3141.9304,
	O	-2.17042398	2.24020369	-0.36965140	3783.0605
	H	-1.66161715	2.58053507	0.38356469	
	C	3.10246454	-0.91647504	-0.63929322	
	H	3.08293761	-2.00346849	-0.74232331	630.4337i, 25.3223, 54.2992, 71.3884,
	H	3.59202709	-0.50783678	-1.52283834	95.4763, 97.7135, 116.7725, 126.9891,
	H	3.71423394	-0.68375032	0.23414731	205.9553, 234.9617, 246.7343,
	C	0.98289065	-0.87796886	0.76739413	280.9598, 310.7543, 407.6885,
	H	0.81344118	-1.95570111	0.65900087	516.9980, 623.6318, 729.9673,
	H	1.64733860	-0.75303274	1.62612888	746.5862, 784.9840, 856.5185,
	C	1.69691820	-0.37463380	-0.47298034	871.5116, 918.6869, 950.4715,
	H	1.74572589	0.76923825	-0.37852536	986.4585, 1038.8828, 1066.4822,
	H	1.10447978	-0.53477368	-1.37522933	1075.0721, 1093.9498, 1116.9431,
	C	-0.34278728	-0.17608931	1.04832350	1164.2911, 1168.3579, 1229.6327,
	H	-0.15053537	0.88805232	1.21072074	1267.2155, 1272.1951, 1301.3366,
	H	-0.75824459	-0.56499921	1.98144186	1307.7663, 1331.7855, 1342.1100,
	C	-1.37958781	-0.33710321	-0.05762543	1375.7806, 1389.0205, 1406.2995,
	H	-1.49579979	-1.39959431	-0.29845508	1409.4764, 1412.0293, 1413.4557,
	H	-1.02996516	0.15068031	-0.97142567	1478.4453, 1487.3576, 1491.0689,
	C	-2.73671751	0.24516182	0.31790736	1498.1256, 1501.0543, 1501.6683,
	H	-3.10173371	-0.25064616	1.22104589	1503.5382, 1513.2078, 1677.1673,
	H	-2.61233614	1.29994127	0.57562932	3023.8042, 3028.3741, 3045.4403,
	C	-3.76385169	0.10484831	-0.79771605	3049.9913, 3050.4820, 3056.6346,
	H	-3.91574253	-0.94455199	-1.05489967	3063.5093, 3071.7407, 3081.0973,
	H	-3.42950587	0.62056365	-1.69900819	3092.9247, 3097.6947, 3113.7575,
	H	-4.72864485	0.52239514	-0.51179206	3122.8088, 3130.1446, 3131.5706,
	O	2.13452314	2.16731774	0.00990597	3785.2887
	H	3.09016425	2.00250237	-0.02892532	
SP2_11	C	3.10246454	-0.91647504	-0.63929322	
	H	3.08293761	-2.00346849	-0.74232331	630.4337i, 25.3223, 54.2992, 71.3884,
	H	3.59202709	-0.50783678	-1.52283834	95.4763, 97.7135, 116.7725, 126.9891,
	H	3.71423394	-0.68375032	0.23414731	205.9553, 234.9617, 246.7343,
	C	0.98289065	-0.87796886	0.76739413	280.9598, 310.7543, 407.6885,
	H	0.81344118	-1.95570111	0.65900087	516.9980, 623.6318, 729.9673,
	H	1.64733860	-0.75303274	1.62612888	746.5862, 784.9840, 856.5185,
	C	1.69691820	-0.37463380	-0.47298034	871.5116, 918.6869, 950.4715,
	H	1.74572589	0.76923825	-0.37852536	986.4585, 1038.8828, 1066.4822,
	H	1.10447978	-0.53477368	-1.37522933	1075.0721, 1093.9498, 1116.9431,
	C	-0.34278728	-0.17608931	1.04832350	1164.2911, 1168.3579, 1229.6327,
	H	-0.15053537	0.88805232	1.21072074	1267.2155, 1272.1951, 1301.3366,
	H	-0.75824459	-0.56499921	1.98144186	1307.7663, 1331.7855, 1342.1100,
	C	-1.37958781	-0.33710321	-0.05762543	1375.7806, 1389.0205, 1406.2995,
	H	-1.49579979	-1.39959431	-0.29845508	1409.4764, 1412.0293, 1413.4557,
	H	-1.02996516	0.15068031	-0.97142567	1478.4453, 1487.3576, 1491.0689,
	C	-2.73671751	0.24516182	0.31790736	1498.1256, 1501.0543, 1501.6683,
	H	-3.10173371	-0.25064616	1.22104589	1503.5382, 1513.2078, 1677.1673,
	H	-2.61233614	1.29994127	0.57562932	3023.8042, 3028.3741, 3045.4403,
	C	-3.76385169	0.10484831	-0.79771605	3049.9913, 3050.4820, 3056.6346,
	H	-3.91574253	-0.94455199	-1.05489967	3063.5093, 3071.7407, 3081.0973,
	H	-3.42950587	0.62056365	-1.69900819	3092.9247, 3097.6947, 3113.7575,
	H	-4.72864485	0.52239514	-0.51179206	3122.8088, 3130.1446, 3131.5706,
	O	2.13452314	2.16731774	0.00990597	3785.2887
	H	3.09016425	2.00250237	-0.02892532	
SP2_12	C	-3.39941845	-0.79704465	-0.09838264	
	H	-3.49708038	-1.84626683	0.18953377	488.8594i, 27.7679, 51.4085, 71.4266,
	H	-4.24421204	-0.25210074	0.31950824	93.8716, 96.6940, 121.6878, 141.3373,
	H	-3.46369022	-0.74265368	-1.18522441	148.2348, 234.7678, 245.4396,
	C	-0.85271992	-0.91246529	-0.19703652	287.2585, 356.3384, 396.3524,
	H	-0.87578815	-1.97587357	0.06775526	494.1508, 621.6749, 735.2628,
	H	-0.90607825	-0.86659426	-1.28869816	766.2225, 809.0482, 865.1371,
	C	-2.07761922	-0.23830667	0.38878021	886.3820, 924.1523, 944.4296,
	H	-2.03837965	0.86232753	0.07004824	985.1109, 1028.6411, 1059.8216,
	H	-2.02843114	-0.22370409	1.48030331	1084.4062, 1094.7576, 1107.6257,
	C	0.45845822	-0.29735030	0.27407161	1161.1960, 1194.9466, 1232.5402,
	H	0.51272776	-0.35065130	1.36701980	1238.9408, 1260.1334, 1298.2965,
	H	0.45717728	0.76270709	0.00971287	1314.6550, 1330.1751, 1342.4186,
	C	1.68085254	-0.98494879	-0.32328118	1346.3583, 1378.5362, 1390.8329,
	H	1.66217898	-0.86258752	-1.41079201	1406.3635, 1410.6505, 1415.6764,
	H	1.61050187	-2.05922401	-0.13267406	1479.5347, 1485.3309, 1492.8476,
	C	3.01065708	-0.46601462	0.21800534	1493.6597, 1499.1577, 1504.9961,
	H	3.04393330	-0.62667036	1.29901739	1507.1622, 1512.5050, 1669.2001,
	H	3.82178321	-1.06074731	-0.20621847	3024.8092, 3028.7895, 3040.3479,

	C	3.25696091	1.00774118	-0.08588292	3047.4696, 3053.3428, 3059.9375,
	H	2.53550439	1.64782177	0.42108767	3061.0197, 3071.4272, 3077.5164,
	H	3.17435235	1.19984650	-1.15714885	3085.7348, 3098.1521, 3118.5740,
	H	4.25193895	1.31536486	0.23392865	3127.1498, 3136.1690, 3141.5338,
	O	-1.86629184	2.32970743	-0.22439914	3784.7700
	H	-1.54913050	2.57168133	0.66039044	
SP2_13	C	2.83196382	1.53453431	-0.23730664	641.6415i, 32.9126, 49.7882, 68.6565,
	H	2.44835198	2.54498904	-0.08224097	87.1848, 102.0914, 116.1178,
	H	3.85453036	1.50550942	0.13776999	127.6418, 207.4981, 234.5928,
	H	2.85407945	1.35682567	-1.31409861	243.8317, 275.4387, 312.7172,
	C	0.52796200	0.45840583	-0.06633092	406.8895, 517.4536, 620.7137,
	H	0.06785435	1.44340350	0.06259839	725.4710, 743.7543, 788.5053,
	H	0.55228052	0.26485005	-1.14376240	853.7526, 872.0300, 921.3335,
	C	1.94874412	0.51798554	0.45741405	949.1746, 988.5745, 1034.4461,
	H	2.39533821	-0.52873253	0.30458845	1058.3786, 1076.5690, 1104.7069,
	H	1.96490249	0.64749298	1.54237856	1111.0349, 1153.9713, 1184.9439,
	C	-0.30900236	-0.61332777	0.62302670	1224.4202, 1259.3933, 1280.4493,
	H	-0.40225661	-0.36590274	1.68517977	1293.9205, 1309.2926, 1331.0341,
	H	0.23355461	-1.55998111	0.56903393	1344.8709, 1370.9044, 1397.3856,
	C	-1.69986143	-0.79299541	0.02236126	1405.8002, 1408.4116, 1410.4406,
	H	-2.20319179	-1.62022502	0.52967718	1413.5089, 1476.8703, 1486.5971,
	H	-1.60447430	-1.09045369	-1.02673050	1496.1086, 1498.2486, 1498.8743,
	C	-2.58476223	0.44593134	0.11037812	1500.9296, 1503.3952, 1511.7720,
	H	-2.61336975	0.79250094	1.14749604	1692.1511, 3028.5697, 3034.8370,
	H	-2.14555934	1.25696275	-0.47401795	3040.8866, 3047.8060, 3050.7493,
	C	-4.00082381	0.17919490	-0.38380804	3057.0068, 3059.2168, 3069.7673,
H	-4.47852010	-0.60051557	0.21104189	3076.4699, 3091.3221, 3093.2368,	
H	-3.99024248	-0.15807656	-1.42135681	3112.4555, 3123.7581, 3131.2465,	
H	-4.62253918	1.07214739	-0.32847993	3131.6310, 3785.6806	
O	2.97753058	-1.75803766	-0.32994807		
H	3.58369620	-1.27486570	-0.91389957		
SP2_14	C	2.83150514	1.53474119	-0.23723440	641.6507i, 32.9289, 49.8221, 68.7402,
	H	2.44771693	2.54510678	-0.08202398	85.5563, 102.1387, 116.1544,
	H	3.85412084	1.50588110	0.13772394	127.6189, 207.5425, 234.5996,
	H	2.85353019	1.35713686	-1.31404466	243.8265, 275.5040, 312.7597,
	C	0.52772154	0.45818855	-0.06607497	406.9118, 517.4656, 620.7474,
	H	0.06745732	1.44311248	0.06292490	725.4943, 743.7761, 788.5039,
	H	0.55191723	0.26465721	-1.14351488	853.7972, 872.0362, 921.3348,
	C	1.94855797	0.51795619	0.45748781	949.2105, 988.6083, 1034.4500,
	H	2.39529589	-0.52866924	0.30445032	1058.3793, 1076.5679, 1104.7252,
	H	1.96484406	0.64732892	1.54246644	1111.0240, 1153.9726, 1184.9504,
	C	-0.30907434	-0.61363451	0.62334267	1224.4362, 1259.4169, 1280.4923,
	H	-0.40256891	-0.36606354	1.68543900	1293.9432, 1309.2984, 1331.0374,
	H	0.23361045	-1.56022505	0.56954576	1344.8886, 1370.8864, 1397.3651,
	C	-1.69978202	-0.79334449	0.02240207	1405.8009, 1408.4073, 1410.4435,
	H	-2.20340713	-1.62037088	0.52975116	1413.5158, 1476.8808, 1486.6162,
	H	-1.60416262	-1.09099302	-1.02661403	1496.1178, 1498.2500, 1498.8842,
	C	-2.58430434	0.44588801	0.10998771	1500.9317, 1503.4050, 1511.7770,
	H	-2.61253781	0.79300105	1.14693504	1692.1538, 3028.5411, 3034.8428,
	H	-2.14488405	1.25645467	-0.47490753	3040.8848, 3047.7951, 3050.7469,
	C	-4.00057247	0.17945268	-0.38378391	3057.0226, 3059.1933, 3069.7660,
H	-4.47842791	-0.59983997	0.21148165	3076.4692, 3091.3034, 3093.2388,	
H	-3.99035291	-0.15822667	-1.42120199	3112.4556, 3123.7731, 3131.2374,	
H	-4.62195291	1.07265219	-0.32868134	3131.6358, 3785.6940	
O	2.97765716	-1.75775622	-0.33034876		
H	3.58423523	-1.27437886	-0.91370156		
SP2_15	C	-3.35575017	-0.77544669	-0.04801642	641.5630i, 33.5222, 43.1115, 77.8583,
	H	-3.45572491	-1.85709134	0.06296229	

	H	-4.19186354	-0.30891461	0.47202380	91.9232, 98.6333, 121.7780, 136.6682,
	H	-3.44110855	-0.54850136	-1.11228462	150.3383, 235.0210, 245.8845,
	C	-0.81578632	-0.86964265	-0.22825019	288.5371, 357.8895, 397.2282,
	H	-0.82728932	-1.96238436	-0.14248573	496.5304, 623.1461, 725.7561,
	H	-0.90399047	-0.64294432	-1.29520722	750.1293, 782.1501, 847.8064,
	C	-2.02155878	-0.30647911	0.49615002	885.5841, 923.0050, 952.0436,
	H	-1.95757064	0.83525456	0.39121111	984.4021, 1027.5595, 1058.3004,
	H	-1.94801759	-0.46963107	1.57408822	1083.6809, 1104.7340, 1110.6482,
	C	0.50611906	-0.32549537	0.29709687	1155.6701, 1183.2971, 1218.7563,
	H	0.60079623	-0.56618003	1.36126352	1257.4567, 1270.7840, 1297.9410,
	H	0.48441685	0.76404172	0.22363308	1313.1050, 1336.1126, 1345.3428,
	C	1.71055921	-0.88073637	-0.45415170	1376.7943, 1385.8963, 1403.2443,
	H	1.65051826	-0.57090044	-1.50231892	1409.4553, 1413.1429, 1416.6240,
	H	1.65671145	-1.97290185	-0.45197584	1476.9313, 1484.7468, 1493.1520,
	C	3.05514514	-0.44411285	0.12228846	1498.3179, 1500.1630, 1504.1663,
	H	3.13055231	-0.79190746	1.15610735	1506.1414, 1512.6860, 1691.0651,
	H	3.85510009	-0.94203994	-0.42898110	3023.9083, 3031.4047, 3040.6848,
	C	3.27492398	1.06400892	0.07500982	3047.1928, 3051.2452, 3059.6182,
	H	2.56736188	1.59245201	0.71299333	3060.6771, 3070.8635, 3078.4629,
	H	3.14897403	1.44032983	-0.94183807	3085.6337, 3099.8333, 3113.2116,
	H	4.27867202	1.32652355	0.40746448	3126.5866, 3130.7815, 3136.7356,
	O	-1.99167549	2.22432439	-0.17593096	3783.3581
	H	-2.83604688	2.10762472	-0.63996915	
	C	-3.26853476	-1.01297749	0.13351344	
	H	-3.21635723	-2.09758140	0.24826270	645.9520i, 30.1112, 48.1492, 80.4074,
	H	-4.09847167	-0.65372263	0.74131937	94.0122, 106.2237, 127.7092,
	H	-3.49357310	-0.80714054	-0.91453343	140.3314, 146.3342, 240.3355,
	C	-0.77054290	-0.78133572	-0.31274480	248.9985, 288.9553, 359.2625,
	H	-0.62986328	-1.86536950	-0.22913697	397.4147, 495.9978, 621.6167,
	H	-0.99995759	-0.57994195	-1.36345483	725.5936, 749.2654, 781.1618,
	C	-1.95614410	-0.37213792	0.53733464	848.6702, 886.1068, 924.0743,
	H	-2.05068041	0.76754863	0.43137661	951.3360, 985.4013, 1027.7098,
	H	-1.75003118	-0.51548927	1.60074561	1060.6902, 1083.2019, 1105.3904,
	C	0.51735923	-0.06560041	0.07271239	1111.1853, 1160.6688, 1175.0048,
	H	0.72803164	-0.25952256	1.12755573	1221.5615, 1259.4655, 1270.6944,
	H	0.36472849	1.01380050	-0.02265443	1299.2295, 1312.9589, 1337.0335,
	C	1.70521041	-0.49065686	-0.78273489	1347.0164, 1378.9334, 1384.1391,
	H	1.43652275	-0.38050734	-1.83667721	1402.5781, 1409.4117, 1413.2603,
	H	1.90002242	-1.55630706	-0.62357836	1416.4518, 1477.7696, 1484.5275,
	C	2.98146779	0.30037619	-0.50659682	1493.2932, 1498.8358, 1500.9060,
	H	3.75563326	-0.02096473	-1.20593596	1504.8547, 1506.1736, 1514.2840,
	H	2.79726220	1.35765194	-0.71391832	1689.9581, 3023.3161, 3032.0568,
	C	3.49659385	0.14393752	0.91999316	3046.6283, 3050.3138, 3051.1726,
	H	3.62922850	-0.91067990	1.16928688	3057.9721, 3059.1922, 3069.6325,
	H	2.80464523	0.57242112	1.64444320	3077.5142, 3086.9408, 3097.2269,
	H	4.45716518	0.64144332	1.04912194	3113.5852, 3125.0439, 3129.5622,
	O	-2.33242583	2.13263626	-0.12433570	3135.7455, 3785.1464
	H	-3.20735562	1.90363940	-0.47639966	
	C	-2.98990625	-1.13073246	-0.67371015	
	H	-2.85675790	-2.21446197	-0.68448309	648.5476i, 28.6505, 55.5520, 73.0032,
	H	-4.03500532	-0.92612350	-0.44320653	78.7816, 94.9409, 117.5046, 133.0644,
	H	-2.78115702	-0.76750051	-1.68165788	205.5515, 240.7768, 243.2850,
	C	-0.58262463	-0.68341131	0.03396286	272.2688, 312.4978, 406.8938,
	H	-0.35363665	-1.75610629	0.04201514	515.9644, 623.1419, 726.2585,
	H	-0.38450415	-0.33086353	-0.98127254	743.8395, 788.2124, 854.8998,
	C	-2.05572435	-0.49062718	0.33300576	870.6327, 922.6207, 947.1701,
	H	-2.23707826	0.64388483	0.33946250	988.4123, 1032.8760, 1058.1032,
	H	-2.29683308	-0.79490327	1.35436365	1079.5829, 1105.2730, 1111.3744,
SP2_16					
SP2_17					

	C	0.31916402	0.04168631	1.02630625	1163.9739, 1171.2803, 1224.6826,
	H	0.03689780	-0.25558517	2.03976820	1268.1092, 1273.3281, 1295.4986,
	H	0.12591285	1.11561540	0.95245948	1311.0615, 1331.6315, 1343.5730,
	C	1.80730408	-0.22579192	0.82144258	1370.2440, 1397.5655, 1404.8742,
	H	2.00556346	-1.29616789	0.93898040	1409.0873, 1410.9273, 1413.9241,
	H	2.37134378	0.27820942	1.61074127	1477.3601, 1486.6853, 1496.6614,
	C	2.34295023	0.23407042	-0.53055179	1498.7546, 1499.1275, 1501.0726,
	H	1.86516316	-0.33431226	-1.33092947	1503.5618, 1512.2997, 1690.2735,
	H	2.06601217	1.28029469	-0.68693033	3019.2823, 3032.9645, 3045.1208,
	C	3.85450507	0.07677197	-0.63481298	3050.5078, 3051.0713, 3056.2144,
	H	4.14559821	-0.96502388	-0.49146944	3065.1859, 3068.5351, 3076.3502,
	H	4.35962328	0.66820120	0.13010166	3093.2019, 3095.2716, 3112.9224,
	H	4.22702434	0.39738454	-1.60712389	3122.9694, 3130.8922, 3131.0018,
	O	-2.42658031	2.06087415	-0.11324565	3784.3748
	H	-3.01953324	1.83867007	-0.84870916	
	C	-2.52823661	-1.73781432	-0.24961868	
	H	-2.00735185	-2.68912421	-0.11954521	483.0545i, 27.4140, 57.6172, 67.3290,
	H	-3.49977926	-1.81554783	0.23551900	92.9818, 121.9643, 132.7240,
	H	-2.69221636	-1.59106673	-1.31730609	149.7534, 197.1721, 236.9952,
	C	-0.36041680	-0.39456737	-0.34114528	279.4230, 292.6979, 383.1290,
	H	0.21875671	-1.31969185	-0.24552063	400.1067, 505.6675, 623.2165,
	H	-0.51066861	-0.23521155	-1.41354184	724.2252, 776.4320, 832.3563,
	C	-1.70548253	-0.60311747	0.32666638	858.3830, 862.6847, 925.1926,
	H	-2.30786708	0.36046843	0.17598889	946.5913, 970.9747, 1033.9490,
	H	-1.58935795	-0.70360695	1.40869869	1039.5490, 1080.1162, 1093.8845,
	C	0.41995557	0.77537859	0.24541682	1118.2425, 1159.6303, 1176.9875,
	H	0.62628855	0.57550850	1.30081248	1233.3788, 1241.5007, 1263.7882,
	H	-0.21530541	1.66396679	0.21699535	1294.5379, 1308.9529, 1331.5080,
	C	1.72381276	1.07686688	-0.49158422	1342.0791, 1361.9321, 1381.5320,
	H	2.22341213	1.91321565	0.00434943	1389.8824, 1407.1483, 1410.9260,
	H	1.48664000	1.41368189	-1.50390825	1414.2150, 1476.8143, 1487.9056,
	C	2.69641540	-0.09971259	-0.57317538	1493.7229, 1495.9155, 1499.7947,
	H	2.27007570	-0.88908565	-1.19615479	1500.2265, 1506.9888, 1517.1689,
	H	3.60156752	0.23216844	-1.08487252	1669.9284, 3028.0584, 3045.1030,
	C	3.06708142	-0.67041300	0.79081177	3046.6362, 3053.6701, 3055.3421,
	H	2.20557065	-1.12514530	1.28133747	3056.9634, 3061.0986, 3073.4694,
	H	3.44520802	0.11405959	1.44914010	3080.4225, 3091.1495, 3095.4068,
	H	3.83763459	-1.43547050	0.70359037	3118.4737, 3121.6559, 3130.9031,
	O	-3.01816369	1.68738565	0.10515394	3141.6961, 3783.7531
	H	-2.82607295	1.95207182	1.01895765	
SP2_18	C	-2.55025120	1.62183472	0.29786806	
	H	-2.05254724	2.59200695	0.35527694	640.5201i, 34.7179, 51.0191, 71.2700,
	H	-3.50006382	1.76527428	-0.21652127	118.9517, 125.0585, 132.1195,
	H	-2.75639056	1.30068216	1.32049036	155.1247, 199.1060, 239.2704,
	C	-0.35836423	0.32205157	0.28467321	281.1183, 294.2471, 384.4738,
	H	0.20891179	1.25609761	0.36458709	403.3288, 506.3887, 626.9802,
	H	-0.56306123	-0.00393985	1.30966563	720.9697, 747.2742, 802.5613,
	C	-1.67073184	0.61410667	-0.41425531	854.3048, 858.7139, 923.3966,
	H	-2.23068135	-0.38592271	-0.48210385	954.0031, 971.7731, 1032.8850,
	H	-1.50891457	0.88985265	-1.45924637	1039.0770, 1075.1311, 1105.9852,
	C	0.46801736	-0.73927014	-0.43174854	1118.0424, 1150.9786, 1176.3868,
	H	0.72876431	-0.37683124	-1.42992065	1213.9680, 1256.4829, 1276.4583,
	H	-0.15663954	-1.62294854	-0.58007671	1294.4288, 1306.8139, 1331.9870,
	C	1.73270838	-1.14452207	0.32307559	1362.2703, 1378.7338, 1389.6065,
	H	2.27167094	-1.88924605	-0.26839048	1399.0897, 1407.8805, 1411.7234,
	H	1.44464759	-1.63831752	1.25466883	1414.5135, 1475.5812, 1488.5174,
	C	2.68130682	0.01046807	0.64416239	1496.4254, 1498.0301, 1500.0539,
	H	2.20934651	0.68893848	1.35842567	1500.7515, 1507.3040, 1517.3914,
SP2_19	C	-2.55025120	1.62183472	0.29786806	
	H	-2.05254724	2.59200695	0.35527694	640.5201i, 34.7179, 51.0191, 71.2700,
	H	-3.50006382	1.76527428	-0.21652127	118.9517, 125.0585, 132.1195,
	H	-2.75639056	1.30068216	1.32049036	155.1247, 199.1060, 239.2704,
	C	-0.35836423	0.32205157	0.28467321	281.1183, 294.2471, 384.4738,
	H	0.20891179	1.25609761	0.36458709	403.3288, 506.3887, 626.9802,
	H	-0.56306123	-0.00393985	1.30966563	720.9697, 747.2742, 802.5613,
	C	-1.67073184	0.61410667	-0.41425531	854.3048, 858.7139, 923.3966,
	H	-2.23068135	-0.38592271	-0.48210385	954.0031, 971.7731, 1032.8850,
	H	-1.50891457	0.88985265	-1.45924637	1039.0770, 1075.1311, 1105.9852,
	C	0.46801736	-0.73927014	-0.43174854	1118.0424, 1150.9786, 1176.3868,
	H	0.72876431	-0.37683124	-1.42992065	1213.9680, 1256.4829, 1276.4583,
	H	-0.15663954	-1.62294854	-0.58007671	1294.4288, 1306.8139, 1331.9870,
	C	1.73270838	-1.14452207	0.32307559	1362.2703, 1378.7338, 1389.6065,
	H	2.27167094	-1.88924605	-0.26839048	1399.0897, 1407.8805, 1411.7234,
	H	1.44464759	-1.63831752	1.25466883	1414.5135, 1475.5812, 1488.5174,
	C	2.68130682	0.01046807	0.64416239	1496.4254, 1498.0301, 1500.0539,
	H	2.20934651	0.68893848	1.35842567	1500.7515, 1507.3040, 1517.3914,

	H	3.56185670	-0.39221179	1.14801018	1691.9210, 3026.4399, 3044.8978,
	C	3.11781321	0.79202792	-0.58955769	3048.7838, 3051.0459, 3055.3566,
	H	2.27752644	1.31239254	-1.05061808	3057.4315, 3061.0523, 3075.4280,
	H	3.54351894	0.12396879	-1.34062552	3080.4128, 3091.6033, 3096.9764,
	H	3.87044350	1.53879693	-0.33926565	3113.2629, 3122.8491, 3130.1785,
	O	-3.02164399	-1.61080835	-0.12609073	3131.0470, 3782.4137
	H	-3.69822747	-1.13230642	0.37906341	
SP2_20	C	-2.62491406	-1.33658087	-0.74959015	498.8828i, 34.3878, 45.3492, 59.8027,
	H	-2.41348888	-2.37585393	-0.48497114	74.4364, 91.2560, 117.0506, 137.8536,
	H	-3.67686831	-1.26399825	-1.02021457	150.8267, 239.5330, 248.3784,
	H	-2.03478890	-1.08981877	-1.63084958	282.9649, 359.4574, 392.1429,
	C	-0.86304710	-0.51155410	0.92460326	494.2736, 647.3909, 728.4884,
	H	-0.74050739	0.18046514	1.76155234	751.2972, 818.4724, 849.2266,
	H	-0.69338884	-1.51714490	1.32652054	895.7897, 921.1544, 943.2183,
	C	-2.29108138	-0.42122619	0.41354601	986.2496, 1025.9940, 1053.5624,
	H	-2.43837954	0.65400273	0.04568685	1080.4496, 1096.1523, 1105.8178,
	H	-3.00350171	-0.55102675	1.22986523	1161.5034, 1190.1716, 1230.5476,
	C	0.19230942	-0.20295145	-0.13135404	1239.9076, 1262.5967, 1301.4995,
	H	-0.04746565	0.75547598	-0.60171413	1327.4987, 1334.0952, 1335.9643,
	H	0.15977950	-0.95705209	-0.92193518	1360.1725, 1376.0184, 1392.7516,
	C	1.60119341	-0.15153198	0.44482643	1410.0935, 1411.4386, 1414.8799,
	H	1.82707760	-1.10120156	0.94087346	1475.6890, 1486.4477, 1492.8361,
	H	1.64635735	0.61753381	1.22228975	1493.3110, 1503.1056, 1503.7227,
	C	2.66846670	0.13309934	-0.60420474	1505.9291, 1513.8594, 1675.9320,
	H	2.62576404	-0.63853506	-1.37721643	3025.0661, 3028.9242, 3044.5572,
	H	2.43707551	1.07840218	-1.10141748	3050.3011, 3052.0831, 3056.3185,
	C	4.07058739	0.19153823	-0.01238636	3056.9119, 3068.7930, 3082.6849,
H	4.32811654	-0.75345290	0.46825376	3085.1543, 3096.6255, 3122.6142,	
H	4.13938080	0.97532107	0.74334940	3122.9189, 3131.0981, 3146.0439,	
H	4.82170887	0.39501198	-0.77483890	3784.9306	
O	-2.54520183	2.13061256	-0.25645561		
H	-3.09634263	2.34221303	0.51376849		
SP2_21	C	2.37212643	1.49697671	-0.34269264	612.4523i, 40.7463, 46.1426, 55.7358,
	H	1.63449283	2.28684259	-0.19442637	106.5047, 113.5822, 123.3332,
	H	3.34678258	1.90623918	-0.07761981	136.6747, 149.6397, 239.9227,
	H	2.37908481	1.24892709	-1.40625882	247.0892, 267.2315, 357.9007,
	C	0.77891793	-0.46084789	0.07877422	396.2026, 480.9067, 640.6990,
	H	0.86923143	-0.76940305	-0.96690899	727.9333, 753.1941, 799.7871,
	H	0.68864986	-1.37765098	0.66559009	843.9903, 886.8673, 919.9660,
	C	2.04155481	0.27377773	0.49148373	948.1043, 989.6107, 1030.6856,
	H	2.90565025	-0.47429234	0.39350245	1053.3386, 1073.1634, 1092.7292,
	H	2.02691449	0.51604571	1.55679857	1115.7361, 1146.1478, 1193.3006,
	C	-0.49117669	0.36971996	0.25335525	1233.3879, 1244.5959, 1271.8477,
	H	-0.45114157	1.25031821	-0.39319258	1297.4552, 1330.2372, 1331.7915,
	H	-0.54179762	0.74258107	1.28144800	1335.0935, 1365.5834, 1391.9773,
	C	-1.75535419	-0.42014307	-0.06051367	1398.4442, 1406.5268, 1408.3705,
	H	-1.80732012	-1.29520606	0.59456356	1413.3633, 1481.1553, 1487.3492,
	H	-1.69563021	-0.80723704	-1.08255920	1493.9025, 1498.9322, 1503.8116,
	C	-3.02991446	0.39997082	0.09325275	1504.0070, 1505.7751, 1514.5966,
	H	-3.08358159	0.79060406	1.11272776	1689.3151, 3031.5160, 3036.6870,
	H	-2.97833397	1.27005599	-0.56634175	3046.7850, 3050.2836, 3051.5138,
	C	-4.28467371	-0.40623682	-0.21563894	3057.8224, 3058.5257, 3070.2279,
H	-4.36734140	-1.26471121	0.45234585	3074.4994, 3087.4787, 3100.3197,	
H	-4.25942365	-0.78533141	-1.23825251	3117.5489, 3123.9183, 3128.1110,	
H	-5.18685356	0.19391495	-0.10303985	3132.7704, 3784.6040	
O	4.05102324	-1.28839189	-0.12713491		
H	4.32355085	-0.64386627	-0.79942133		
SP2_22	C	2.32065677	1.62094645	-0.29260992	460.3858i, 27.6498, 32.9724, 54.4711,

	H	1.58204258	2.36043352	0.02123784	91.2675, 116.4486, 120.1108,
	H	3.30497112	1.99624947	-0.01681448	135.7594, 146.8754, 231.8468,
	H	2.27968826	1.54486784	-1.37986363	246.8913, 291.5164, 358.4846,
	C	0.77753375	-0.41789903	-0.11706200	388.9194, 492.0255, 625.7767,
	H	0.81600465	-0.54808612	-1.20227202	725.8967, 753.3320, 830.6390,
	H	0.73322376	-1.42037368	0.31499778	862.0872, 890.0999, 921.6904,
	C	2.04810813	0.27299534	0.34739935	949.0833, 980.4412, 1033.8786,
	H	2.91788969	-0.41339313	0.06339338	1052.1225, 1084.2803, 1097.0311,
	H	2.07365018	0.34286191	1.43768841	1107.2197, 1160.7150, 1196.9941,
	C	-0.49430623	0.34193318	0.25485849	1225.2126, 1238.4098, 1268.7835,
	H	-0.49698199	1.32033956	-0.23244015	1295.0505, 1329.3132, 1331.0798,
	H	-0.50004504	0.53304224	1.33291764	1335.4364, 1343.6338, 1367.8628,
	C	-1.76138721	-0.40969251	-0.13231391	1392.5875, 1405.2618, 1409.6581,
	H	-1.76982649	-1.38579586	0.36252651	1413.6173, 1481.5579, 1486.0781,
	H	-1.74670249	-0.61290778	-1.20767656	1493.1052, 1497.2946, 1499.8339,
	C	-3.03766076	0.34399263	0.21981294	1503.7640, 1505.1638, 1513.5546,
	H	-3.04832404	0.54832191	1.29359191	1696.5222, 3030.5759, 3036.0440,
	H	-3.02774793	1.31728462	-0.27747684	3047.5587, 3050.4488, 3056.4211,
	C	-4.29548866	-0.42071365	-0.17110905	3057.3603, 3059.4895, 3066.0829,
	H	-4.33562397	-1.38561612	0.33626473	3073.9707, 3086.9571, 3100.3640,
	H	-4.31434734	-0.61174744	-1.24498591	3121.8482, 3123.7374, 3131.9353,
	H	-5.19867940	0.13111570	0.08687458	3138.0400, 3786.3400
	O	4.12719939	-1.29394332	-0.14219339	
	H	4.36847865	-1.35442460	0.79572846	
	C	1.74144951	-1.13814003	1.26264689	
	H	1.78007353	-2.22157133	1.12167324	561.2532i, 45.4804, 52.8809, 93.3547,
	H	2.48528655	-0.86668740	2.00932080	107.2471, 134.6340, 174.8917,
	H	0.75832270	-0.89252309	1.66490156	179.4247, 221.9910, 249.9770,
	C	1.07385546	-0.80623373	-1.19466683	288.2946, 308.5176, 350.0521,
	H	1.26103514	-0.14017070	-2.04113658	444.1244, 526.5143, 659.4833,
	H	1.34889477	-1.81149737	-1.52936313	753.6265, 776.6449, 800.2339,
	C	2.00229971	-0.42549686	-0.04979466	841.1188, 853.2026, 908.7432,
	H	1.93858059	0.70527708	0.15193094	953.8671, 972.7727, 1013.9710,
	H	3.04154268	-0.54313930	-0.35967186	1047.3637, 1067.4910, 1097.3917,
	C	-0.41526416	-0.79574296	-0.85598374	1128.7085, 1156.6856, 1170.7185,
	H	-0.61418143	-1.53886139	-0.08133097	1207.5086, 1235.6157, 1262.3975,
	H	-0.97930655	-1.11543431	-1.73644545	1273.0132, 1311.7287, 1317.1134,
	C	-0.93420675	0.56644812	-0.40726434	1343.3025, 1369.1173, 1378.8143,
	H	-0.64581522	1.31287088	-1.15632593	1382.2124, 1405.7440, 1412.5920,
	H	-0.45160349	0.85181556	0.53294706	1415.3088, 1477.9267, 1488.9301,
	C	-2.44847895	0.61400672	-0.21548408	1491.1899, 1493.2599, 1500.8673,
	H	-2.74369689	1.63655186	0.02647865	1510.8505, 1512.7038, 1517.8551,
	H	-2.93822259	0.36539668	-1.16055180	1622.2227, 3019.4279, 3035.3331,
	C	-2.94383216	-0.32400726	0.87999659	3049.6597, 3050.0503, 3053.6597,
	H	-2.41728814	-0.13364400	1.81734585	3058.8655, 3067.5823, 3074.1537,
	H	-2.78530254	-1.36897238	0.61546907	3088.7077, 3090.7565, 3100.8266,
	H	-4.00928902	-0.18911271	1.06195191	3116.8880, 3125.9699, 3137.6703,
	O	1.92868482	2.18559715	0.33438799	3143.0107, 3784.3768
	H	1.08655536	2.31992071	-0.12899628	
SP2_23	C	-1.85807909	-0.98098413	1.16849289	
	H	-1.05397740	-1.62085520	1.53654023	616.8895i, 42.6549, 56.0443, 66.8165,
	H	-2.40306296	-0.60915080	2.03597756	100.3788, 110.5978, 132.8172,
	H	-2.53092156	-1.60707843	0.57873381	187.7143, 210.4598, 255.3412,
	C	-0.67839174	-0.27271450	-0.98486328	264.1643, 308.1190, 364.2582,
	H	-1.44454733	-0.74702485	-1.60275923	425.6110, 523.9602, 637.5760,
	H	-0.34845003	0.61277334	-1.53033239	724.9662, 759.3109, 801.1987,
	C	-1.30927014	0.15675411	0.32898134	844.6664, 880.8807, 896.8100,
	H	-2.17457790	0.85971075	0.05715575	949.5210, 962.6375, 1035.8907,
SP2_24	C	-1.85807909	-0.98098413	1.16849289	
	H	-1.05397740	-1.62085520	1.53654023	616.8895i, 42.6549, 56.0443, 66.8165,
	H	-2.40306296	-0.60915080	2.03597756	100.3788, 110.5978, 132.8172,
	H	-2.53092156	-1.60707843	0.57873381	187.7143, 210.4598, 255.3412,
	C	-0.67839174	-0.27271450	-0.98486328	264.1643, 308.1190, 364.2582,
	H	-1.44454733	-0.74702485	-1.60275923	425.6110, 523.9602, 637.5760,
	H	-0.34845003	0.61277334	-1.53033239	724.9662, 759.3109, 801.1987,
	C	-1.30927014	0.15675411	0.32898134	844.6664, 880.8807, 896.8100,
	H	-2.17457790	0.85971075	0.05715575	949.5210, 962.6375, 1035.8907,

	H	-0.63870426	0.79016713	0.91407365	1048.1862, 1060.0360, 1080.2436,
	C	0.49492952	-1.24462145	-0.81504878	1128.2199, 1148.3698, 1163.3917,
	H	0.92071253	-1.44511691	-1.80134538	1228.3712, 1237.4289, 1263.8393,
	H	0.12075915	-2.20119023	-0.44370572	1305.9120, 1323.7745, 1330.9361,
	C	1.60024487	-0.74334805	0.11200591	1351.7162, 1372.6571, 1387.2378,
	H	2.39159655	-1.49615178	0.15640207	1400.1978, 1407.3530, 1410.8210,
	H	1.21820663	-0.64844917	1.13337889	1413.2130, 1484.0349, 1491.3666,
	C	2.20984489	0.58738286	-0.31500890	1492.1521, 1498.8013, 1502.9510,
	H	2.52879953	0.51637010	-1.35874648	1504.8525, 1509.6182, 1512.4340,
	H	1.44952762	1.37095141	-0.27989602	1682.9077, 3037.4666, 3048.6770,
	C	3.38951602	0.98897525	0.56087219	3049.0450, 3051.1419, 3056.5015,
	H	4.18160343	0.24053072	0.51189847	3060.0826, 3068.7105, 3076.9314,
	H	3.08336627	1.07727729	1.60445566	3083.9869, 3092.2123, 3106.6020,
	H	3.81157823	1.94527026	0.25428516	3114.2479, 3122.2452, 3127.5305,
	O	-3.52253878	1.41022227	-0.28638333	3132.7602, 3784.2762
	H	-4.02436422	0.73152370	0.19236235	
	C	2.21914931	1.59276712	-0.61088463	496.3111i, 29.1550, 43.7484, 67.6441,
	H	1.95463954	2.53478105	-0.12362696	80.3101, 88.1707, 107.2179, 141.3026,
	H	3.21869022	1.69771905	-1.02922121	165.6505, 253.0963, 266.5063,
	H	1.52592044	1.43755810	-1.43612903	309.5281, 320.7162, 459.6469,
	C	0.82555301	0.27588041	1.09712995	463.8396, 643.5451, 733.4221,
	H	0.90443806	-0.55753546	1.79962755	768.8250, 813.1534, 843.0744,
	H	0.62470830	1.17005955	1.69871329	889.3324, 912.5341, 948.8525,
	C	2.15734823	0.45129424	0.38693524	973.3397, 1019.0538, 1031.8248,
	H	2.34526557	-0.51544864	-0.19910934	1079.6290, 1099.8773, 1109.5748,
	H	2.97382096	0.51888356	1.10777607	1157.2346, 1186.2052, 1228.5368,
	C	-0.34855943	0.02364593	0.15782629	1232.7381, 1266.9555, 1303.1021,
	H	-0.10377211	-0.81869463	-0.49734768	1318.5373, 1334.3115, 1355.0120,
	H	-0.49321158	0.89290312	-0.48620214	1370.9949, 1378.5026, 1381.2153,
	C	-1.64003437	-0.27351525	0.91162017	1408.2379, 1411.8835, 1415.3252,
	H	-1.90798197	0.59534307	1.52189260	1475.4102, 1484.6281, 1491.8484,
	H	-1.45929531	-1.09582879	1.60884922	1493.0209, 1503.8878, 1504.9880,
	C	-2.81633223	-0.63460200	0.00774746	1507.0090, 1512.6390, 1677.0521,
	H	-2.56193853	-1.52807872	-0.56823334	3023.7717, 3030.9394, 3046.8553,
	H	-3.67182164	-0.90232345	0.63081086	3049.3878, 3052.4277, 3057.7254,
	C	-3.22033027	0.48634961	-0.94376627	3068.9497, 3073.5360, 3084.8482,
	H	-2.43607117	0.69736710	-1.67009389	3086.5656, 3103.2600, 3123.1350,
	H	-3.42070617	1.40729977	-0.39273934	3124.5808, 3135.2727, 3146.6235,
	H	-4.12082476	0.22642208	-1.49915716	3783.1953
	O	2.54432607	-1.88978629	-0.79438481	
	H	3.21276609	-2.17305685	-0.15038028	
SP2_25	C	2.21914931	1.59276712	-0.61088463	496.3111i, 29.1550, 43.7484, 67.6441,
	H	1.95463954	2.53478105	-0.12362696	80.3101, 88.1707, 107.2179, 141.3026,
	H	3.21869022	1.69771905	-1.02922121	165.6505, 253.0963, 266.5063,
	H	1.52592044	1.43755810	-1.43612903	309.5281, 320.7162, 459.6469,
	C	0.82555301	0.27588041	1.09712995	463.8396, 643.5451, 733.4221,
	H	0.90443806	-0.55753546	1.79962755	768.8250, 813.1534, 843.0744,
	H	0.62470830	1.17005955	1.69871329	889.3324, 912.5341, 948.8525,
	C	2.15734823	0.45129424	0.38693524	973.3397, 1019.0538, 1031.8248,
	H	2.34526557	-0.51544864	-0.19910934	1079.6290, 1099.8773, 1109.5748,
	H	2.97382096	0.51888356	1.10777607	1157.2346, 1186.2052, 1228.5368,
	C	-0.34855943	0.02364593	0.15782629	1232.7381, 1266.9555, 1303.1021,
	H	-0.10377211	-0.81869463	-0.49734768	1318.5373, 1334.3115, 1355.0120,
	H	-0.49321158	0.89290312	-0.48620214	1370.9949, 1378.5026, 1381.2153,
	C	-1.64003437	-0.27351525	0.91162017	1408.2379, 1411.8835, 1415.3252,
	H	-1.90798197	0.59534307	1.52189260	1475.4102, 1484.6281, 1491.8484,
	H	-1.45929531	-1.09582879	1.60884922	1493.0209, 1503.8878, 1504.9880,
	C	-2.81633223	-0.63460200	0.00774746	1507.0090, 1512.6390, 1677.0521,
	H	-2.56193853	-1.52807872	-0.56823334	3023.7717, 3030.9394, 3046.8553,
	H	-3.67182164	-0.90232345	0.63081086	3049.3878, 3052.4277, 3057.7254,
	C	-3.22033027	0.48634961	-0.94376627	3068.9497, 3073.5360, 3084.8482,
	H	-2.43607117	0.69736710	-1.67009389	3086.5656, 3103.2600, 3123.1350,
	H	-3.42070617	1.40729977	-0.39273934	3124.5808, 3135.2727, 3146.6235,
	H	-4.12082476	0.22642208	-1.49915716	3783.1953
	O	2.54432607	-1.88978629	-0.79438481	
	H	3.21276609	-2.17305685	-0.15038028	
	C	-1.94026072	1.43751485	0.82999125	617.7057i, 36.7279, 50.9985, 55.9210,
	H	-1.29960144	2.31335817	0.71358231	96.5474, 114.9819, 137.5550,
	H	-2.96416598	1.78779170	0.94888636	168.2145, 223.6223, 248.3694,
	H	-1.64860890	0.92590627	1.74866807	272.7541, 298.6653, 356.4392,
	C	-0.46021591	-0.17021720	-0.49437890	433.5214, 516.1700, 649.7354,
	H	-0.25726365	-0.73505174	0.42120827	727.2816, 768.2119, 797.5410,
	H	-0.49192394	-0.89475970	-1.31386142	848.6787, 854.1672, 909.3304,
	C	-1.81294379	0.50738084	-0.36047423	953.6132, 969.6091, 1019.8850,
	H	-2.61012028	-0.30740744	-0.23361823	1046.2736, 1058.9391, 1104.4213,
	H	-2.09344583	1.00622271	-1.29120849	1118.6693, 1145.9948, 1169.0501,
	C	0.68049309	0.81404771	-0.74975882	1227.9378, 1243.8187, 1269.6619,
	H	0.79990617	1.46712003	0.11711324	1304.9118, 1317.8114, 1332.5840,
	H	0.40684555	1.46317406	-1.58584520	1367.2221, 1377.0105, 1388.2885,
	C	2.01026070	0.13031599	-1.06414935	1390.5938, 1399.5191, 1410.9133,
	H	2.77324563	0.89845757	-1.21506387	1415.7482, 1479.2188, 1490.4478,
	H	1.91851299	-0.40763673	-2.01123577	
SP2_26	C	-1.94026072	1.43751485	0.82999125	617.7057i, 36.7279, 50.9985, 55.9210,
	H	-1.29960144	2.31335817	0.71358231	96.5474, 114.9819, 137.5550,
	H	-2.96416598	1.78779170	0.94888636	168.2145, 223.6223, 248.3694,
	H	-1.64860890	0.92590627	1.74866807	272.7541, 298.6653, 356.4392,
	C	-0.46021591	-0.17021720	-0.49437890	433.5214, 516.1700, 649.7354,
	H	-0.25726365	-0.73505174	0.42120827	727.2816, 768.2119, 797.5410,
	H	-0.49192394	-0.89475970	-1.31386142	848.6787, 854.1672, 909.3304,
	C	-1.81294379	0.50738084	-0.36047423	953.6132, 969.6091, 1019.8850,
	H	-2.61012028	-0.30740744	-0.23361823	1046.2736, 1058.9391, 1104.4213,
	H	-2.09344583	1.00622271	-1.29120849	1118.6693, 1145.9948, 1169.0501,
	C	0.68049309	0.81404771	-0.74975882	1227.9378, 1243.8187, 1269.6619,
	H	0.79990617	1.46712003	0.11711324	1304.9118, 1317.8114, 1332.5840,
	H	0.40684555	1.46317406	-1.58584520	1367.2221, 1377.0105, 1388.2885,
	C	2.01026070	0.13031599	-1.06414935	1390.5938, 1399.5191, 1410.9133,
	H	2.77324563	0.89845757	-1.21506387	1415.7482, 1479.2188, 1490.4478,
	H	1.91851299	-0.40763673	-2.01123577	

	C	2.49313222	-0.83876380	0.01519059	1494.4102, 1497.0171, 1500.1362,
	H	1.81794823	-1.69553034	0.07143522	1501.3127, 1507.7524, 1517.9645,
	H	3.46273138	-1.23895821	-0.28614139	1686.4120, 3030.7607, 3043.1994,
	C	2.61655913	-0.19492457	1.39142752	3051.9009, 3055.2063, 3056.5882,
	H	1.64344546	0.10630370	1.78167318	3059.0238, 3063.2472, 3076.2694,
	H	3.24435711	0.69699719	1.34707296	3080.8980, 3092.2553, 3100.3596,
	H	3.06070480	-0.88207354	2.11047659	3119.0884, 3122.4447, 3131.8726,
	O	-3.34106777	-1.56062231	0.14309094	3139.6985, 3784.9523
	H	-2.55617348	-2.13105816	0.12504230	
SP2_27	C	2.39189412	-1.17592080	0.83673588	612.6234i, 39.0901, 47.9159, 62.5644,
	H	1.85672884	-2.12493398	0.89319090	90.9918, 95.5742, 124.8617, 138.4869,
	H	3.45794449	-1.40200899	0.82234897	233.5964, 238.6145, 266.3091,
	H	2.16864270	-0.61775030	1.74849916	270.8325, 303.5540, 407.6572,
	C	0.54231940	0.10913536	-0.37206733	527.8974, 639.1638, 735.6344,
	H	0.40365504	0.75118839	0.50111241	767.3226, 794.1974, 844.4536,
	H	0.36429916	0.73427123	-1.25081436	870.2905, 905.7929, 950.4279,
	C	1.97708634	-0.38643753	-0.39038602	969.5815, 1039.7449, 1050.5963,
	H	2.64647621	0.54190443	-0.46727393	1064.4538, 1092.4944, 1119.5711,
	H	2.19230225	-0.94128454	-1.30669978	1143.6736, 1184.2851, 1230.0631,
	C	-0.48040412	-1.02819061	-0.35203032	1245.4897, 1283.4539, 1305.3250,
	H	-0.42406376	-1.55428052	0.60480551	1315.1886, 1334.5445, 1343.7066,
	H	-0.21437326	-1.75684417	-1.12307755	1366.6217, 1393.3691, 1400.1843,
	C	-1.91456584	-0.55714202	-0.57751935	1403.6725, 1409.6273, 1413.6335,
	H	-2.57683007	-1.42675319	-0.60255418	1480.0985, 1488.2506, 1496.8704,
	H	-1.98974755	-0.08445259	-1.56181283	1498.5607, 1501.8452, 1503.5393,
	C	-2.42123161	0.41585253	0.48165605	1505.0249, 1512.3970, 1691.0713,
	H	-2.26722344	-0.02184162	1.47227622	3034.3729, 3040.0509, 3047.9814,
	H	-1.82913889	1.33255134	0.45368033	3050.9140, 3052.3210, 3057.0694,
	C	-3.89306049	0.75904493	0.29143962	3068.4342, 3068.6511, 3075.8534,
H	-4.51198669	-0.13709254	0.35405435	3094.2568, 3101.1679, 3117.1801,	
H	-4.06106886	1.20806978	-0.68859063	3124.0764, 3127.4958, 3132.1044,	
H	-4.24327197	1.46251718	1.04591083	3784.1132	
O	3.50088742	1.72891124	-0.13963607		
H	3.80832971	1.38739915	0.71506202		
SP2_28	C	2.09841226	1.66249296	-0.45201916	622.4353i, 30.1515, 56.1062, 60.6448,
	H	1.23591034	2.33118546	-0.44180047	96.5527, 114.0507, 116.0588,
	H	2.96775703	2.23644118	-0.13571143	130.5723, 159.9937, 238.9906,
	H	2.26213822	1.33902065	-1.48092260	275.3996, 305.6549, 318.6404,
	C	0.78410865	-0.48708904	-0.00844687	448.0272, 463.3576, 656.0486,
	H	1.02377450	-0.84816330	-1.01429375	735.9874, 756.2655, 784.3018,
	H	0.76790341	-1.36255412	0.64700913	844.3273, 880.5230, 910.1514,
	C	1.87204959	0.46731292	0.45251775	955.7064, 980.1996, 1034.3595,
	H	2.86113345	-0.11241078	0.49220953	1038.9113, 1070.3689, 1105.5417,
	H	1.70694154	0.77380610	1.48816462	1112.7617, 1143.2874, 1187.6427,
	C	-0.60936078	0.13823355	-0.02505265	1227.6781, 1245.5685, 1277.5440,
	H	-0.63831126	0.95858876	-0.74766808	1302.4270, 1319.1300, 1333.4720,
	H	-0.81019793	0.57872481	0.95514686	1362.0125, 1378.3147, 1380.7829,
	C	-1.69405587	-0.87423297	-0.37677927	1388.8539, 1403.6508, 1412.1736,
	H	-1.72997110	-1.64413743	0.40042876	1415.1055, 1481.5818, 1486.2894,
	H	-1.41254055	-1.38356971	-1.30235066	1493.3723, 1495.1710, 1500.1535,
	C	-3.08252164	-0.26191752	-0.54363433	1504.7780, 1507.8350, 1512.2156,
	H	-3.05565606	0.46904144	-1.35607993	1681.5193, 3029.0780, 3034.1009,
	H	-3.77816524	-1.04314528	-0.85543376	3047.0895, 3049.5934, 3056.8397,
	C	-3.60884811	0.40362086	0.72317702	3059.0144, 3062.5506, 3070.2852,
H	-3.00922995	1.27064344	0.99904065	3078.7351, 3087.3897, 3098.3994,	
H	-3.59030160	-0.29438277	1.56230173	3120.6857, 3126.0827, 3135.8605,	
H	-4.63589163	0.74254103	0.59285683	3140.3647, 3784.1040	
O	3.98259885	-1.06603891	0.21370451		

	H	3.41521147	-1.77384280	-0.13110833	
SP2_29	C	-1.48450735	1.54054021	-0.00214690	
	H	-0.46315108	1.91751667	-0.08585563	619.2429i, 35.3813, 47.5997, 67.2986,
	H	-2.11658535	2.16806646	-0.63021446	99.4905, 103.8402, 135.1918,
	H	-1.79527110	1.66560084	1.03728640	160.5058, 227.9941, 234.4032,
	C	-0.85118798	-0.88108295	0.51710827	285.4128, 298.9121, 357.2475,
	H	-1.34794742	-0.85677036	1.49005355	431.5785, 515.2365, 632.3268,
	H	-0.96330001	-1.89711437	0.13268057	735.5832, 773.0598, 802.7571,
	C	-1.56446253	0.08382608	-0.41662493	847.9585, 855.7435, 909.1165,
	H	-2.66745073	-0.23278385	-0.42527934	947.9075, 965.5923, 1022.0183,
	H	-1.25209873	-0.04871807	-1.45407480	1043.5861, 1059.4512, 1096.4007,
	C	0.63661495	-0.57158163	0.70140410	1126.2579, 1148.0961, 1164.0946,
	H	1.07066177	-1.32026134	1.36993393	1227.4009, 1233.8193, 1273.3812,
	H	0.74548101	0.38946140	1.20856538	1307.0797, 1316.6298, 1334.6206,
	C	1.41924236	-0.55981000	-0.60786836	1356.8133, 1376.4751, 1384.4179,
	H	1.08161817	0.27430537	-1.23101386	1392.4154, 1405.4580, 1412.7496,
	H	1.18874163	-1.47240547	-1.16504141	1415.5996, 1480.8890, 1490.7652,
	C	2.92978589	-0.44954715	-0.41651034	1493.2581, 1494.2166, 1501.1361,
H	3.28174305	-1.30745173	0.16240635	1505.3722, 1512.1598, 1513.0305,	
H	3.41691501	-0.51399515	-1.39116125	1685.6165, 3034.1236, 3047.9729,	
C	3.35615157	0.84113891	0.27467858	3048.8268, 3049.8885, 3056.6766,	
H	2.99619329	0.88282761	1.30233186	3057.2522, 3069.7851, 3079.4965,	
H	2.95810751	1.71047022	-0.25291496	3087.1953, 3094.1645, 3104.4212,	
H	4.44108291	0.93521328	0.30217066	3112.4560, 3123.9385, 3126.2130,	
O	-4.12471603	-0.35806100	-0.11085672	3136.7358, 3787.8161	
H	-4.22683316	0.54962561	0.21673833		
SP2_30	C	2.10903820	1.52890402	-0.46463551	
	H	1.26824848	2.22386140	-0.47545676	609.7762i, 32.3602, 43.6531, 68.7944,
	H	2.99242120	2.09000030	-0.16027094	102.6994, 106.8264, 117.6141,
	H	2.25836562	1.17702999	-1.48762581	131.4449, 167.8110, 251.6581,
	C	0.73277669	-0.57025957	0.02899933	280.9466, 301.3270, 320.2802,
	H	0.97464393	-0.97470782	-0.95822400	446.7056, 466.7186, 637.6110,
	H	0.68747148	-1.42286170	0.71039142	735.3470, 761.8556, 801.4108,
	C	1.84517140	0.36375037	0.47019471	843.3930, 879.7016, 909.3716,
	H	2.79943420	-0.26930971	0.53725714	956.1856, 974.8557, 1023.9446,
	H	1.68840752	0.70873517	1.49494833	1036.7832, 1072.5847, 1104.6279,
	C	-0.63916061	0.10044414	-0.02071509	1115.9949, 1142.2868, 1186.8945,
	H	-0.63808722	0.89576545	-0.77179648	1224.8244, 1245.7283, 1277.8528,
	H	-0.83476514	0.58094115	0.94176398	1301.1587, 1317.0774, 1331.7053,
	C	-1.75255977	-0.88928155	-0.34708635	1355.6957, 1379.0812, 1383.0580,
	H	-1.81855412	-1.62981206	0.45605486	1397.7360, 1402.9262, 1409.5535,
	H	-1.47899066	-1.43959216	-1.25115969	1416.0979, 1480.6338, 1485.9149,
	C	-3.11965114	-0.24032335	-0.54830173	1493.5915, 1499.5662, 1504.4492,
H	-3.06362859	0.46000443	-1.38595591	1505.3485, 1507.5420, 1512.7775,	
H	-3.83700015	-1.01020732	-0.83850449	1689.4318, 3035.1966, 3040.8081,	
C	-3.63509603	0.48634620	0.68910199	3047.8982, 3049.1156, 3052.3702,	
H	-3.01066020	1.34366282	0.93915195	3058.4051, 3067.2362, 3072.7080,	
H	-3.64466421	-0.18127518	1.55273631	3082.5662, 3088.4236, 3101.0613,	
H	-4.65005159	0.85201783	0.53772039	3118.2503, 3125.4217, 3127.9068,	
O	4.08735633	-0.96754380	0.22231348	3135.4145, 3786.1847	
H	4.36544644	-0.34138364	-0.46488211		
SP3_1	C	-3.61038672	-0.34437990	0.28702098	
	H	-3.67360237	0.70840065	0.01014846	477.1113i, 35.3759, 50.6550, 64.7552,
	H	-4.49075258	-0.85290822	-0.10358749	85.8293, 91.4346, 101.1574, 142.9729,
	H	-3.64220536	-0.40792486	1.37584125	161.3491, 242.5796, 249.8906,
	C	-1.08394399	-0.26100811	0.27256845	252.4284, 307.8561, 425.0448,
	H	-1.16283916	0.83623285	-0.04918375	486.5438, 618.7685, 731.5539,
H	-1.08088905	-0.24136944	1.36671825	769.3307, 786.5420, 870.6493,	

	C	-2.32478673	-0.95660333	-0.25262482	900.1591, 930.3338, 946.9013,
	H	-2.27179302	-2.01641515	0.01606296	1020.9362, 1027.0528, 1063.3426,
	H	-2.32063416	-0.91421470	-1.34413679	1085.5308, 1092.0143, 1102.0283,
	C	0.23281296	-0.78407819	-0.26549582	1170.5614, 1202.2813, 1216.1582,
	H	0.21412148	-0.74737405	-1.35846466	1247.2532, 1266.9629, 1297.5440,
	H	0.33067793	-1.84147622	0.00586594	1311.3114, 1328.3156, 1334.9144,
	C	1.44044381	-0.01203585	0.24906707	1347.8101, 1374.1044, 1397.7849,
	H	1.45698631	-0.05233160	1.34312908	1407.9073, 1412.7605, 1414.3317,
	H	1.32882542	1.04211994	-0.02140855	1478.5848, 1488.3142, 1490.9329,
	C	2.76354529	-0.53795049	-0.29221705	1501.4215, 1502.2589, 1503.9537,
	H	2.86770754	-1.59299747	-0.02561832	1509.8180, 1513.7503, 1678.8106,
	H	2.74382203	-0.49756026	-1.38421005	3024.8084, 3033.3556, 3040.1976,
	C	3.96065841	0.24561403	0.22969967	3048.1828, 3052.1832, 3057.1614,
	H	4.01118209	0.19624590	1.31842463	3058.5247, 3062.4503, 3073.9200,
	H	3.88584049	1.29730516	-0.05005821	3084.7259, 3092.1518, 3123.5570,
	H	4.89891921	-0.14081410	-0.16672586	3126.3047, 3132.1471, 3136.7462,
	O	-1.26838949	2.31503047	-0.35834121	3782.6531
	H	-1.21830907	2.60748888	0.56582196	
	C	3.25680301	0.22174301	-0.25701063	657.0633i, 43.8786, 80.5453, 99.7402,
	H	2.98012953	1.27460598	-0.30370485	117.5739, 123.3622, 149.0111,
	H	4.21451148	0.14131553	0.25551481	193.0387, 239.3744, 256.1898,
	H	3.39176408	-0.13565295	-1.27891463	288.1033, 301.5867, 389.4194,
	C	0.82794497	-0.48226098	-0.23151619	403.7716, 492.6273, 666.6259,
	H	0.58951833	0.64502031	-0.26224254	712.8473, 741.6672, 805.1026,
	H	0.89933468	-0.76298946	-1.28742907	843.4596, 863.0404, 926.0240,
	C	2.17602070	-0.57948687	0.45606427	941.2637, 970.6635, 1031.7456,
	H	2.46460950	-1.63391700	0.51266754	1041.8700, 1073.7401, 1094.7231,
	H	2.07096735	-0.23047348	1.48618850	1115.4228, 1148.7572, 1176.0401,
	C	-0.28983269	-1.23513266	0.46527521	1186.3587, 1247.1642, 1270.1618,
	H	-0.46531194	-0.79109801	1.44865222	1293.5841, 1303.2501, 1325.9368,
	H	0.06022307	-2.25395172	0.65931180	1356.5471, 1368.4871, 1383.3411,
	C	-1.59059819	-1.31332290	-0.33280015	1392.7327, 1407.1465, 1413.4446,
	H	-2.31531258	-1.91184966	0.22536827	1415.7699, 1477.4412, 1485.1367,
	H	-1.39487309	-1.85121957	-1.26377619	1492.8019, 1502.5418, 1504.5529,
	C	-2.21841029	0.03922103	-0.66474731	1509.3830, 1510.4623, 1521.9032,
	H	-1.52140907	0.62702788	-1.26738273	1616.4435, 3035.7348, 3040.1796,
	H	-3.09326573	-0.12436613	-1.29610861	3046.4706, 3050.3920, 3054.0045,
	C	-2.64241783	0.82342229	0.57352967	3058.3724, 3062.1890, 3074.1674,
	H	-1.80520557	1.00758748	1.24963939	3082.1837, 3087.4752, 3093.9163,
	H	-3.38973522	0.26772203	1.14191436	3118.6614, 3125.3708, 3129.8631,
	H	-3.07892923	1.78633794	0.30679187	3142.2271, 3780.1184
	O	0.47106676	2.12258386	-0.05536180	
	H	-0.49260784	2.12013253	0.06363505	
	C	2.83141967	-0.15109722	1.06404041	490.5207i, 49.3320, 67.3322, 77.3920,
	H	2.70267754	0.93133728	1.10508242	88.4002, 118.8053, 131.0148,
	H	3.16071197	-0.48793373	2.04604338	202.9397, 214.1855, 250.7974,
	H	3.62688834	-0.37067783	0.35009321	263.7763, 295.0318, 318.5237,
	C	1.05943101	-0.37105090	-0.72193854	426.0745, 501.9921, 641.6633,
	H	0.84957545	0.75542441	-0.65340217	739.7593, 770.0443, 801.6406,
	H	1.87068945	-0.45787572	-1.44928702	850.6609, 884.5998, 904.2528,
	C	1.52878154	-0.82135685	0.64882215	942.1714, 973.1171, 1048.7508,
	H	1.65233551	-1.90955969	0.63558328	1055.0429, 1066.9117, 1072.1203,
	H	0.75561677	-0.60821527	1.38949160	1121.3056, 1164.8603, 1173.8116,
	C	-0.19747650	-1.04601808	-1.25129693	1204.6085, 1250.3561, 1264.0655,
	H	0.04755521	-2.08786610	-1.48228282	1293.6230, 1310.1107, 1315.7155,
	H	-0.47686771	-0.57692460	-2.19772703	1331.5605, 1343.6135, 1380.4601,
	C	-1.39227119	-1.00998833	-0.30113737	1396.1148, 1409.6276, 1411.2171,
	H	-1.17176137	-1.59317512	0.59750260	
SP3_2					
SP3_3					

	H	-2.23643858	-1.50959548	-0.78352153	1413.1572, 1477.9747, 1482.8828,
	C	-1.81360292	0.39844352	0.10316412	1489.6380, 1499.5442, 1503.6393,
	H	-1.00616573	0.88605421	0.65327169	1504.2049, 1509.4363, 1513.0262,
	H	-1.96478727	1.00081792	-0.79645744	1727.8825, 3033.5580, 3036.7191,
	C	-3.07959776	0.39637974	0.94979786	3044.1543, 3053.5641, 3057.0786,
	H	-2.93545419	-0.18726309	1.86065563	3058.6234, 3066.6303, 3069.4748,
	H	-3.91347283	-0.04695021	0.40333218	3083.2344, 3089.0712, 3096.5606,
	H	-3.36808292	1.40536683	1.24189104	3121.3028, 3125.0037, 3132.2258,
	O	0.87822793	2.26464664	-0.60879773	3135.3064, 3783.8114
	H	1.76105386	2.36799181	-0.99859743	
SP3_4	C	-3.32215986	0.09577554	0.69026616	475.3830i, 31.1291, 53.1090, 78.2761,
	H	-3.26823225	1.11617167	0.30882962	89.1954, 92.3512, 106.1466, 151.7039,
	H	-4.34658670	-0.25530700	0.57408723	216.1946, 242.9176, 255.8289,
	H	-3.09648407	0.12268781	1.75750973	271.3750, 310.2088, 412.2831,
	C	-0.90134833	-0.32882194	0.09765512	516.7241, 615.1342, 738.5169,
	H	-0.84555111	0.73215814	-0.33788080	772.0645, 807.1849, 865.1240,
	H	-0.64141054	-0.21759756	1.15333794	885.6570, 921.4643, 945.4590,
	C	-2.33575778	-0.79797118	-0.04914444	990.8647, 1040.1307, 1057.2658,
	H	-2.40673020	-1.82460711	0.32445898	1071.9432, 1096.7226, 1111.4872,
	H	-2.59122343	-0.83795636	-1.11033092	1164.1713, 1195.6254, 1216.8623,
	C	0.12888762	-1.16330165	-0.64187821	1251.3319, 1273.7426, 1294.5324,
	H	-0.23858927	-1.36404803	-1.65088873	1301.9435, 1310.2951, 1327.6569,
	H	0.21137237	-2.13505267	-0.14174684	1342.4624, 1373.6512, 1400.0549,
	C	1.50782447	-0.51364968	-0.72599350	1407.8247, 1412.2716, 1412.7826,
	H	1.42962027	0.41048215	-1.30500559	1479.4376, 1485.7401, 1489.5165,
	H	2.18032154	-1.17579472	-1.27738551	1496.3140, 1503.6227, 1503.9708,
	C	2.12939336	-0.19585604	0.62937378	1509.3472, 1511.5620, 1715.2996,
	H	1.52288007	0.55321500	1.14336307	3026.9773, 3039.1021, 3039.5053,
H	2.11286548	-1.09254793	1.25609695	3049.3307, 3057.5782, 3057.8252,	
C	3.55690704	0.31924122	0.49899035	3063.6678, 3073.1219, 3079.8608,	
H	3.58513756	1.22000965	-0.11567649	3092.0377, 3095.2002, 3124.8974,	
H	4.19583292	-0.42565727	0.02270793	3125.3754, 3131.8822, 3136.4916,	
H	3.98905491	0.56103766	1.46943167	3783.0783	
O	-0.71345352	2.20235893	-0.66541241		
H	-0.66712848	2.50143755	0.25677550		
SP3_5	C	3.07206213	-0.69366390	-0.64844676	483.1972i, 34.8407, 56.5667, 72.1624,
	H	3.25711868	0.37281582	-0.77966318	89.5385, 94.8803, 134.9884, 161.3875,
	H	4.01281595	-1.17389194	-0.38276793	205.3877, 253.7287, 272.9537,
	H	2.74888207	-1.09674900	-1.60930687	293.2550, 383.8381, 408.2841,
	C	0.69491438	-0.23994936	0.08118239	506.6060, 622.5361, 728.8922,
	H	0.92319344	0.88165524	-0.00754625	781.4079, 803.0488, 854.1876,
	H	0.35450978	-0.53739234	-0.91452591	867.1971, 925.9662, 962.9671,
	C	2.00852858	-0.91944370	0.41771259	970.5756, 1032.4606, 1037.8442,
	H	1.82465203	-1.99125765	0.54514178	1074.7727, 1098.5073, 1116.9796,
	H	2.36230981	-0.55096880	1.38323862	1161.9574, 1171.7581, 1236.8550,
	C	-0.39895618	-0.40539220	1.11849813	1245.8940, 1264.9455, 1298.6320,
	H	0.01525706	-0.19470509	2.10694334	1305.9258, 1312.1383, 1328.5023,
	H	-0.70848165	-1.45554723	1.13511995	1363.6960, 1383.4817, 1388.8249,
	C	-1.61190815	0.49563804	0.88726044	1405.9315, 1414.1154, 1415.4687,
	H	-1.30536737	1.53312386	1.03907793	1478.8055, 1486.7683, 1491.7196,
	H	-2.36542858	0.27509378	1.64748495	1496.6556, 1503.9452, 1504.8165,
	C	-2.25157353	0.35751754	-0.49402688	1508.9025, 1514.0369, 1677.4490,
	H	-3.11372103	1.02461429	-0.54676692	3035.2783, 3039.9930, 3046.8642,
H	-1.55522488	0.70360297	-1.26298953	3049.9333, 3057.4721, 3059.5084,	
C	-2.69137913	-1.06597015	-0.81620261	3063.5488, 3078.8647, 3083.9123,	
H	-3.35166780	-1.45085763	-0.03693570	3090.1802, 3095.7906, 3122.7926,	
H	-1.83808550	-1.74127199	-0.88827520	3127.2655, 3132.9892, 3137.5090,	
H	-3.22789028	-1.11073452	-1.76310884		

	O	1.08247792	2.36413649	-0.25297217	3777.5360
	H	0.37717623	2.42696071	-0.91720674	
SP3_6	C	-3.39885661	-0.85850283	0.18044447	
	H	-3.68770786	0.16176956	-0.07405767	473.8533i, 33.4664, 51.2043, 65.3573,
	H	-4.12785231	-1.53785839	-0.25918558	89.8459, 99.8306, 114.8324, 138.2084,
	H	-3.45453411	-0.96371189	1.26512210	158.1295, 237.7195, 254.4300,
	C	-0.95592311	-0.21574185	0.27954660	287.7242, 359.8140, 396.4509,
	H	-1.26622799	0.84941936	-0.00745091	496.0383, 622.3298, 741.1783,
	H	-0.99239795	-0.24189454	1.37307022	771.1582, 789.3084, 874.5784,
	C	-1.99003558	-1.14911643	-0.31918103	884.6751, 923.1511, 949.8660,
	H	-1.71199923	-2.18007460	-0.07852510	984.3854, 1030.9951, 1054.3339,
	H	-1.95588151	-1.06586687	-1.40780895	1081.6705, 1099.6538, 1108.1289,
	C	0.46227346	-0.40820033	-0.22020927	1162.6759, 1194.1368, 1210.4443,
	H	0.47592476	-0.31373589	-1.31050331	1246.1136, 1274.1851, 1294.7487,
	H	0.77264290	-1.43318875	0.00638141	1306.9619, 1330.9552, 1334.7872,
	C	1.44359105	0.58687058	0.38927377	1361.3853, 1378.5888, 1392.3969,
	H	1.48815366	0.42715898	1.47159271	1403.2449, 1411.3876, 1415.5253,
	H	1.05079740	1.59500860	0.23667390	1477.0848, 1487.1488, 1492.1770,
	C	2.85281507	0.49903998	-0.19040497	1498.1581, 1503.0224, 1505.4781,
H	2.81060320	0.70701339	-1.26269402	1509.9425, 1512.0901, 1683.2120,	
H	3.46595778	1.28664111	0.25130858	3030.9503, 3036.9118, 3040.1315,	
C	3.52396205	-0.85034864	0.04123574	3050.8035, 3052.0875, 3057.7702,	
H	3.00860014	-1.65060604	-0.48948979	3058.1661, 3068.3386, 3083.7114,	
H	3.52652689	-1.10333634	1.10325861	3086.6780, 3093.4484, 3124.8278,	
H	4.55762966	-0.84132540	-0.30269236	3125.6006, 3134.3863, 3135.4843,	
O	-1.71157062	2.27424185	-0.26760794	3783.3794	
H	-1.89462831	2.48665007	0.66163186		
SP3_7	C	-3.02476896	0.15638954	-0.44997714	
	H	-2.77317633	1.21227491	-0.54865405	608.2959i, 52.6061, 83.2535, 89.5203,
	H	-3.65054815	-0.12782087	-1.29493892	126.9464, 129.7528, 176.2764,
	H	-3.61310931	0.03597587	0.46059199	190.2838, 245.7848, 270.9584,
	C	-0.85792161	-0.28168426	0.76632580	289.7035, 317.8186, 369.8890,
	H	-0.56406632	0.81930898	0.57484340	428.2936, 530.3371, 678.9533,
	H	-1.43384736	-0.20683539	1.69179474	731.7226, 749.6937, 797.7751,
	C	-1.75607800	-0.68360124	-0.38848951	842.6392, 879.0726, 892.6528,
	H	-2.00804325	-1.74463334	-0.28230065	943.1073, 962.3012, 1014.9039,
	H	-1.20904177	-0.59125238	-1.32919207	1044.1667, 1061.4706, 1073.6045,
	C	0.37429201	-1.14606617	0.98130371	1109.0539, 1141.7234, 1163.4940,
	H	0.03551551	-2.12183825	1.34419913	1182.5853, 1233.0087, 1258.1958,
	H	0.97652580	-0.72314919	1.78784770	1296.4350, 1302.3275, 1315.7925,
	C	1.23929711	-1.36952256	-0.26011785	1332.0169, 1365.9492, 1384.6665,
	H	0.67062852	-1.93988517	-0.99724378	1395.6565, 1406.7814, 1412.9591,
	H	2.09148154	-1.99463100	0.01885118	1415.3034, 1480.1240, 1485.7192,
	C	1.75506410	-0.08734238	-0.91061997	1498.6533, 1502.3740, 1503.7185,
H	2.32194024	-0.34960815	-1.80546038	1509.2504, 1510.9047, 1522.3966,	
H	0.91016895	0.51479416	-1.25355030	1631.0207, 3031.1889, 3038.0747,	
C	2.64324139	0.73902626	0.01452497	3051.1381, 3054.2266, 3061.4421,	
H	3.52138627	0.16765497	0.31946035	3061.7544, 3071.2234, 3080.7338,	
H	2.12238625	1.02792332	0.92979862	3087.7153, 3090.4844, 3099.9796,	
H	2.99391868	1.64768078	-0.47580739	3117.9828, 3124.2209, 3130.4967,	
O	-0.39992186	2.27129254	0.26728356	3139.7428, 3777.5300	
H	0.56849928	2.24050543	0.20379194		
SP3_8	C	-3.48866064	-0.55971450	-0.01966128	
	H	-3.60459875	0.48081475	-0.32421748	478.5842i, 34.3109, 45.4907, 64.1474,
	H	-4.24292197	-1.15241779	-0.53543349	90.8062, 94.4276, 112.6676, 137.7713,
	H	-3.68932402	-0.62004285	1.05110885	159.9857, 242.3862, 252.1158,
	C	-1.01216968	-0.23040116	0.36349870	286.6644, 359.1426, 396.8294,
	H	-1.14264044	0.84919453	0.00095452	497.0882, 619.6389, 742.6952,

	H	-1.18948589	-0.19511709	1.44273490	775.7634, 784.9832, 861.9459,
	C	-2.08125976	-1.04892594	-0.33403223	889.8382, 926.6642, 954.2971,
	H	-1.97151733	-2.09603384	-0.03429001	986.1891, 1026.8202, 1055.4513,
	H	-1.90672731	-1.01636444	-1.41184733	1080.5666, 1100.8326, 1107.8667,
	C	0.41771771	-0.63033511	0.05869592	1164.0432, 1193.0241, 1219.1251,
	H	0.56087274	-0.62661246	-1.02420663	1244.1518, 1266.9070, 1298.0314,
	H	0.57571988	-1.66372958	0.39014966	1309.6769, 1324.7832, 1336.8990,
	C	1.44156757	0.28021198	0.72732368	1362.8852, 1378.2410, 1390.9784,
	H	1.21667390	0.33677928	1.79615569	1405.0069, 1413.6104, 1416.2683,
	H	1.32241862	1.29193414	0.32817732	1477.3432, 1487.2730, 1492.4748,
	C	2.88776896	-0.17262777	0.54355660	1498.7575, 1502.9671, 1506.2410,
	H	3.54122739	0.49749772	1.10517297	1509.8306, 1513.4408, 1675.0193,
	H	3.01224288	-1.16536327	0.98447929	3021.5877, 3038.3286, 3040.4402,
	C	3.33333582	-0.20298596	-0.91442749	3047.4184, 3052.3514, 3058.8976,
	H	3.15952908	0.76346830	-1.39083537	3059.6281, 3072.6024, 3081.7454,
	H	2.78958213	-0.95610639	-1.48408692	3086.1123, 3095.9554, 3126.8352,
	H	4.39518348	-0.43199964	-0.99711419	3127.0613, 3134.9513, 3136.4816,
	O	-1.31403520	2.30674652	-0.37318333	3783.4540
	H	-1.30375259	2.63879724	0.53884151	
	C	-2.91536984	-0.83497468	-0.86072789	
	H	-2.26017955	-1.50753070	-1.41330053	484.6652i, 44.9254, 47.9850, 59.1336,
	H	-3.92765134	-1.23114632	-0.92812671	76.0130, 93.2260, 124.6783, 136.2514,
	H	-2.89620172	0.13685727	-1.35628703	149.9285, 242.8740, 245.3689,
	C	-1.13205665	-0.00873227	0.75395173	287.5360, 359.3876, 398.1964,
	H	-1.24069853	1.02678919	0.27732722	490.1291, 647.3367, 730.5462,
	H	-0.91031695	0.17493346	1.80817749	769.5914, 776.0789, 852.5780,
	C	-2.47813722	-0.69606354	0.59314237	893.1820, 922.2911, 953.9005,
	H	-3.22997244	-0.13097268	1.14618928	988.4096, 1023.8173, 1052.2840,
	H	-2.42487780	-1.68392178	1.06209694	1080.8616, 1095.9704, 1107.7043,
	C	0.04471823	-0.67984656	0.07147990	1161.5169, 1193.7501, 1220.7100,
	H	-0.13278773	-0.72940130	-1.00526390	1253.2946, 1258.9884, 1302.8190,
	H	0.11479521	-1.71605994	0.42344881	1316.2335, 1332.5640, 1337.2417,
	C	1.36374948	0.03725995	0.32630782	1363.4177, 1376.3428, 1394.3984,
	H	1.55142473	0.08259901	1.40398722	1408.5887, 1413.4057, 1416.7625,
	H	1.27564681	1.07209588	-0.01901499	1479.3965, 1484.8751, 1489.9072,
	C	2.55034531	-0.62415365	-0.36269262	1500.0229, 1503.0470, 1504.1601,
	H	2.63050740	-1.66051392	-0.02432832	1511.4875, 1512.7770, 1677.5851,
	H	2.36083827	-0.66571097	-1.43816683	3022.4380, 3031.6840, 3038.3184,
	C	3.86050297	0.10625926	-0.09914127	3048.5315, 3057.2909, 3061.1462,
	H	4.07890720	0.13727411	0.96934033	3063.3911, 3068.2952, 3082.4706,
	H	3.80752074	1.13588683	-0.45559975	3089.2100, 3094.9587, 3123.5798,
	H	4.69906962	-0.37811928	-0.59809120	3132.2577, 3133.0789, 3138.2252,
	O	-1.29570042	2.40923683	-0.34923386	3781.7731
	H	-0.89293433	2.86455534	0.40756261	
	C	2.66471327	0.08299356	0.97394027	
	H	2.29287225	-0.60637013	1.73187331	602.5361i, 43.8998, 78.9614, 93.9829,
	H	3.74356761	0.16168882	1.10062644	112.0721, 135.5674, 147.3915,
	H	2.22687437	1.06457756	1.16115531	212.2024, 246.8359, 256.5458,
	C	0.81864083	-0.37887787	-0.71080589	282.6620, 309.5110, 364.4423,
	H	0.51216472	0.73029944	-0.65996486	446.4784, 514.7019, 671.3578,
	H	0.60894774	-0.65799226	-1.74692273	725.3377, 762.2404, 800.6923,
	C	2.31212412	-0.38855668	-0.43209012	839.5725, 854.6148, 912.1160,
	H	2.80862432	0.24829416	-1.16558649	945.0831, 961.3193, 1010.6581,
	H	2.69102078	-1.40351186	-0.59034214	1041.1834, 1063.0571, 1093.7640,
	C	-0.02633259	-1.19783683	0.24905537	1112.3699, 1150.1233, 1156.0406,
	H	0.00180075	-0.75002711	1.24435401	1183.2880, 1244.9352, 1266.0855,
	H	0.43943136	-2.18376860	0.35387306	1296.5127, 1313.5749, 1322.9396,
	C	-1.47307991	-1.38218937	-0.20637109	1347.1420, 1363.5035, 1379.9734,
SP3_9					
SP3_10					

	H	-1.99988269	-2.00429579	0.52190018	1392.1846, 1406.2565, 1412.5486,
	H	-1.47626176	-1.93508964	-1.14901704	1416.4378, 1479.8216, 1483.3448,
	C	-2.24589244	-0.07748802	-0.39451378	1492.9093, 1502.8235, 1505.3702,
	H	-1.76626522	0.52071862	-1.17339458	1509.1995, 1511.2718, 1521.9695,
	H	-3.24438544	-0.31004605	-0.76819707	1635.4262, 3033.1989, 3038.6039,
	C	-2.37357725	0.73436602	0.89091920	3047.2322, 3052.4349, 3057.9771,
	H	-1.39923888	1.00007605	1.30599075	3061.4251, 3066.1238, 3080.3180,
	H	-2.89795068	0.16144379	1.65728295	3089.0024, 3092.3368, 3098.2109,
	H	-2.93304130	1.65586249	0.72692452	3118.1154, 3123.8508, 3131.9131,
	O	0.35932615	2.21937569	-0.57010370	3136.8100, 3776.6719
	H	-0.54246325	2.19867019	-0.21052976	
	C	-3.21396034	-0.81820994	-0.59774855	481.3268i, 39.2270, 51.0267, 68.0554,
	H	-3.38372559	0.20686769	-0.92998700	75.6761, 90.9852, 102.7859, 122.9099,
	H	-3.59451940	-1.48847611	-1.36727052	210.2454, 243.0715, 248.2000,
	H	-3.79907567	-0.98089979	0.30872582	266.1526, 314.6427, 409.1911,
	C	-1.18644684	-0.11972793	0.73284044	505.7897, 652.5257, 730.1888,
	H	-1.28387494	0.94439870	0.32122917	763.1415, 782.1267, 861.9330,
	H	-1.82077493	-0.14819173	1.62248211	881.9764, 917.9868, 939.8940,
	C	-1.73158313	-1.04812033	-0.33670235	988.9096, 1038.7846, 1057.2397,
	H	-1.55995748	-2.08318182	-0.02261395	1072.8550, 1096.2656, 1111.1647,
	H	-1.17191596	-0.90703166	-1.26252046	1161.9968, 1189.7791, 1216.4007,
	C	0.27537211	-0.30766320	1.10094058	1259.5011, 1280.4070, 1297.9598,
	H	0.40728274	-1.30765890	1.52994407	1306.7456, 1326.0506, 1336.5872,
	H	0.53747271	0.40242304	1.88903058	1367.6555, 1376.0398, 1400.1912,
	C	1.23687550	-0.12664721	-0.06841519	1409.2714, 1410.5854, 1411.9348,
	H	1.02106286	0.82586535	-0.56255334	1478.2136, 1484.4770, 1489.7056,
	H	1.07037205	-0.90868541	-0.81373229	1500.3242, 1502.2858, 1502.7107,
	C	2.69792590	-0.15865230	0.36208164	1508.5180, 1513.1357, 1682.6649,
	H	2.87287909	0.63527086	1.09254158	3024.5532, 3036.1459, 3039.0120,
	H	2.90013550	-1.10108542	0.87827102	3048.8823, 3057.3656, 3057.8176,
	C	3.65596410	0.00175017	-0.81088149	3062.8001, 3068.8192, 3076.2338,
	H	3.48197305	0.94806107	-1.32474945	3091.8450, 3098.9379, 3124.1861,
	H	3.51591351	-0.79931459	-1.53809414	3126.0357, 3132.4523, 3134.9966,
	H	4.69596555	-0.01803709	-0.48698009	3780.5371
	O	-1.50458465	2.33684824	-0.24460664	
	H	-2.25741986	2.54851435	0.33043957	
SP3_11	C	2.87478508	-0.13976867	1.05362318	554.0777i, 50.4451, 72.7417, 97.9204,
	H	2.76742539	0.94503668	1.07564091	108.0273, 134.0086, 191.9873,
	H	3.18154454	-0.47365175	2.04390372	193.8161, 206.8213, 253.4819,
	H	3.67524836	-0.38145560	0.35330878	261.9260, 289.6244, 316.3104,
	C	1.11315390	-0.31262033	-0.74188849	424.4362, 526.6085, 664.5445,
	H	0.97054544	0.82592139	-0.66318813	747.9830, 762.6791, 801.3306,
	H	1.92907720	-0.39098445	-1.46435422	845.6207, 882.8670, 890.7995,
	C	1.56625065	-0.79020084	0.62464709	945.0462, 974.0032, 1048.9300,
	H	1.67466507	-1.88009236	0.59795974	1058.0339, 1068.2877, 1074.0265,
	H	0.79196835	-0.57787806	1.36514127	1129.5699, 1163.0724, 1175.4463,
	C	-0.14227586	-0.96761555	-1.29808404	1227.7635, 1241.0224, 1263.0007,
	H	0.11412715	-1.99004806	-1.59291141	1289.9676, 1305.1699, 1314.9088,
	H	-0.43555830	-0.45135780	-2.21612425	1326.8427, 1339.1090, 1384.0880,
	C	-1.33396192	-1.01967378	-0.34441897	1394.1398, 1409.4562, 1414.1164,
	H	-1.08844559	-1.63703245	0.52391908	1414.7248, 1479.0677, 1483.7846,
	H	-2.16259347	-1.52371817	-0.84819654	1496.4862, 1501.5519, 1503.4733,
	C	-1.81000167	0.34588154	0.13765373	1504.5825, 1509.4892, 1521.8456,
	H	-1.01735772	0.82861676	0.71473580	1633.3889, 3024.0668, 3032.3087,
	H	-2.00505827	0.98198187	-0.73315952	3035.9627, 3049.4737, 3058.4576,
	C	-3.06860096	0.25090343	0.99059125	3061.2858, 3067.7996, 3070.6318,
	H	-2.89077278	-0.37289547	1.86765581	3076.2695, 3085.2296, 3093.3594,
	H	-3.88679006	-0.19790610	0.42603281	3124.8533, 3129.8944, 3134.4813,
SP3_12					

	H	-3.39597649	1.23014222	1.33752709	3138.3749, 3782.8904
	O	0.83860469	2.31864571	-0.58011388	
	H	-0.12698168	2.31472078	-0.67972240	
SP3_13	C	-2.93990899	-0.64603019	-0.88993187	610.8792i, 50.8220, 64.1682, 68.6931, 92.7096, 110.2468, 126.0377, 148.8832, 162.3191, 243.5343, 251.9394, 279.6752, 357.6208, 396.2171, 495.4067, 642.7993, 734.9349, 767.9999, 789.7076, 851.0065, 887.2225, 921.4860, 942.0298, 987.4042, 1027.9689, 1052.1423, 1083.0823, 1096.4880, 1109.3944, 1160.8563, 1172.1999, 1217.6839, 1255.0794, 1258.1408, 1298.1774, 1317.2470, 1333.0572, 1335.3376, 1366.3167, 1387.5241, 1407.4120, 1411.5089, 1415.4840, 1416.8066, 1483.9310, 1485.2158, 1490.7665, 1502.1198, 1504.3812, 1506.2838, 1509.7256, 1514.5442, 1653.3464, 3023.2551, 3036.8987, 3038.2447, 3048.2978, 3053.9025, 3058.4518, 3061.8264, 3067.0774, 3077.2542, 3091.0396, 3092.7050, 3125.4280, 3129.9697, 3132.0656, 3137.1397, 3778.2625
	H	-2.27872339	-1.18894600	-1.56494635	
	H	-3.94058560	-1.05960647	-1.00721637	
	H	-2.97028400	0.39812175	-1.20605824	
	C	-1.12278946	-0.09852398	0.81191906	
	H	-1.22547808	1.02231613	0.57080024	
	H	-0.88093264	-0.10360732	1.87769662	
	C	-2.47263695	-0.74725998	0.55739244	
	H	-3.21441661	-0.28623490	1.21092091	
	H	-2.41165590	-1.80023390	0.85117759	
	C	0.03932992	-0.64541015	0.00389096	
	H	-0.14368645	-0.49638098	-1.06455433	
	H	0.09414276	-1.73052943	0.15061897	
	C	1.37353693	-0.01204011	0.37792600	
	H	1.57693230	-0.19985431	1.43659588	
	H	1.29798070	1.07449188	0.27127650	
	C	2.53793903	-0.52788904	-0.45761103	
	H	2.60170644	-1.61423371	-0.35358893	
H	2.33584310	-0.33298728	-1.51420387		
C	3.86546222	0.10589713	-0.06321147		
H	4.09819101	-0.10234191	0.98197844		
H	3.82766179	1.18945768	-0.18289477		
H	4.68750168	-0.27051746	-0.67091404		
O	-1.27087621	2.36108199	-0.10695925		
H	-0.97278365	2.03996825	-0.97325875		
SP3_14	C	2.85303637	1.58617644	0.06412975	467.0786i, 43.7007, 57.7347, 68.9116, 83.1614, 92.4381, 105.4022, 128.0964, 212.7133, 242.2646, 252.6737, 284.4825, 308.5770, 407.3495, 512.3131, 630.1536, 732.1863, 767.0546, 783.9881, 868.1449, 892.6421, 919.4175, 944.7446, 994.0224, 1039.0084, 1056.3958, 1073.8937, 1093.9043, 1111.2196, 1159.9023, 1194.9495, 1223.0491, 1243.6892, 1290.5721, 1296.2245, 1309.0924, 1329.1494, 1333.9295, 1339.1317, 1369.7719, 1393.7502, 1403.7463, 1410.8613, 1413.6261, 1484.0171, 1487.0997, 1491.5971, 1501.8600, 1503.0543, 1503.6281, 1511.0952, 1514.1922, 1683.1748, 3033.1473, 3045.4384, 3046.5463, 3051.6532, 3056.0095, 3057.0404, 3057.5918, 3066.3658, 3081.4520, 3086.8096, 3099.9258, 3123.9127, 3124.4897, 3132.1342, 3136.4927, 3783.7127
	H	3.58490041	0.83610865	-0.23721469	
	H	3.12927426	2.53360274	-0.39665168	
	H	2.92032330	1.70923227	1.14658137	
	C	1.03052202	-0.14593334	0.32044872	
	H	1.83734056	-0.92260071	0.07758468	
	H	1.04636129	-0.04460464	1.40991622	
	C	1.45079784	1.15264419	-0.34297888	
	H	0.73475937	1.93618587	-0.08018889	
	H	1.39675413	1.03207699	-1.42783088	
	C	-0.28865744	-0.73293668	-0.14982298	
	H	-0.42914223	-1.71401943	0.30970482	
	H	-0.24420875	-0.89880097	-1.22984743	
	C	-1.49477214	0.14620351	0.17591631	
	H	-1.40957314	1.10242585	-0.34689204	
	H	-1.49704776	0.37800517	1.24607898	
	C	-2.81749136	-0.50947506	-0.20140603	
	H	-2.80352510	-0.75425907	-1.26651024	
H	-2.91085924	-1.45958239	0.33044366		
C	-4.01761208	0.37546754	0.10864860		
H	-3.95545434	1.31817334	-0.43679563		
H	-4.06010863	0.61190750	1.17282541		
H	-4.95476000	-0.10820992	-0.16449707		
O	2.98737338	-1.88934717	-0.08860368		
H	3.42103948	-1.67374347	0.75250996		
SP3_15	C	-2.91647093	-1.57518868	0.02179048	634.6607i, 45.7049, 58.7443, 66.5676, 86.1275, 94.5253, 123.1841, 132.0043, 185.9355, 240.2242, 247.6494, 277.9249, 302.4222, 402.3404,
	H	-3.64069190	-0.76893228	-0.09518990	
	H	-3.23772418	-2.41637130	-0.59092321	
	H	-2.93466907	-1.89339048	1.06512230	
	C	-1.05914365	0.07227516	0.47443424	

	H	-1.88959491	0.86294223	0.41537292	506.1095, 649.9750, 730.0955,
	H	-1.03398289	-0.19559138	1.53509059	745.5307, 786.9604, 854.2605,
	C	-1.52480126	-1.09725754	-0.37190403	872.5813, 914.6800, 944.4597,
	H	-0.81055855	-1.91971780	-0.27604890	1005.5038, 1040.6647, 1054.8255,
	H	-1.51685530	-0.79778132	-1.42346513	1075.6766, 1087.5928, 1113.4931,
	C	0.24598901	0.71783532	0.04406643	1146.9459, 1190.4297, 1235.0924,
	H	0.41971909	1.61705588	0.64130335	1249.5142, 1288.0217, 1296.8715,
	H	0.16234708	1.04225378	-0.99884030	1311.3793, 1330.9585, 1338.6761,
	C	1.45650000	-0.20347815	0.17912229	1368.8430, 1386.7041, 1400.4819,
	H	1.33587549	-1.07090345	-0.47475863	1406.0588, 1411.9175, 1413.2547,
	H	1.50239923	-0.59107305	1.20189311	1483.1639, 1485.1133, 1490.4019,
	C	2.76888975	0.49393224	-0.15668735	1501.0287, 1502.4130, 1503.5954,
	H	2.71229561	0.89239399	-1.17301171	1510.3522, 1513.1546, 1703.4931,
	H	2.89683985	1.35491215	0.50423751	3027.9623, 3038.3334, 3043.2802,
	C	3.97079558	-0.43330733	-0.03344690	3049.7217, 3056.7164, 3058.0894,
	H	3.87355340	-1.28558218	-0.70732193	3060.9834, 3063.8023, 3075.8389,
	H	4.05664271	-0.82298164	0.98182504	3083.0864, 3095.9785, 3124.6847,
	H	4.90074284	0.08009671	-0.27485058	3129.1264, 3132.9039, 3138.9942,
	O	-2.79400995	1.95453360	-0.08841838	3782.3884
	H	-2.09480993	2.42753514	-0.56733841	
	C	-2.99903886	-1.55254508	0.15292806	
	H	-2.96269984	-1.69415458	1.23435113	472.1500i, 46.8913, 59.0653, 65.8896,
	H	-4.01323411	-1.76965093	-0.18009110	69.8198, 96.3013, 120.3110, 138.8749,
	H	-2.33565960	-2.28685999	-0.30289051	158.7777, 240.0529, 250.5398,
	C	-1.22690503	0.25609989	0.31682541	294.1599, 355.0762, 398.0342,
	H	-1.06450174	1.35536982	0.03503813	494.1350, 629.0745, 735.2482,
	H	-1.21908086	0.23390213	1.41080293	767.8433, 781.0315, 866.6516,
	C	-2.59509809	-0.12780102	-0.22100620	893.9101, 922.4402, 966.2864,
	H	-2.59418033	-0.01830602	-1.30778342	985.7115, 1028.3644, 1052.2480,
	H	-3.33719423	0.57368307	0.16265989	1080.9039, 1095.8990, 1111.4649,
	C	-0.05456778	-0.52633267	-0.24372710	1161.3005, 1195.2920, 1221.6641,
	H	-0.10144307	-0.51123214	-1.33684875	1248.7906, 1268.5433, 1296.9726,
	H	-0.14365980	-1.57553997	0.05656937	1322.9280, 1323.7278, 1338.0508,
	C	1.29536780	0.00901306	0.21639152	1344.8824, 1367.2715, 1393.3489,
	H	1.32646310	0.01897736	1.31114381	1406.1996, 1409.8973, 1413.5430,
	H	1.39456753	1.04886307	-0.10874287	1481.2721, 1491.2812, 1491.5179,
	C	2.47346176	-0.79991971	-0.31093139	1501.5225, 1502.7944, 1503.7699,
	H	2.37094110	-1.83860792	0.01379833	1510.8559, 1514.0136, 1671.4782,
	H	2.43590340	-0.81420840	-1.40311080	3028.3461, 3034.8843, 3048.7906,
	C	3.81526969	-0.24640294	0.15019699	3051.9317, 3057.2475, 3059.9054,
	H	3.88076865	-0.24628975	1.23925934	3060.8147, 3064.8242, 3075.9905,
	H	3.94656572	0.78203031	-0.18894870	3091.6154, 3099.4117, 3124.0069,
	H	4.64722812	-0.83488933	-0.23489100	3129.4228, 3131.7057, 3137.9881,
	O	-0.77011294	2.81872883	-0.17932938	3783.7788
	H	-0.32081746	2.95441342	0.67025548	
	C	-2.51324118	-1.38316280	-0.54100788	
	H	-3.34347186	-1.17074685	0.13468889	477.8107i, 38.5935, 62.6107, 82.6278,
	H	-2.92652924	-1.78000345	-1.46739877	107.4430, 119.0176, 140.8231,
	H	-1.90587846	-2.16532018	-0.08508723	192.6900, 214.6382, 255.0429,
	C	-1.18294757	0.51591336	0.47972232	286.9522, 306.0119, 369.2655,
	H	-0.58060801	1.44322123	0.18039967	432.6747, 510.8183, 633.9409,
	H	-2.01885678	0.89785836	1.07115814	743.3477, 767.3951, 806.0330,
	C	-1.69009308	-0.12394742	-0.80278477	841.9154, 882.1112, 907.2366,
	H	-0.84628420	-0.36388058	-1.45275813	949.0813, 962.8848, 1026.5608,
	H	-2.29563756	0.60426202	-1.34451343	1052.2667, 1061.4459, 1071.9560,
	C	-0.28199088	-0.35114078	1.34988929	1116.5262, 1162.0714, 1169.0840,
	H	-0.89143466	-1.13390097	1.81157611	1200.1765, 1249.5048, 1266.1398,
	H	0.10164429	0.25968023	2.17060078	1290.8767, 1316.2192, 1329.9728,
SP3_16					
SP3_17					

	C	0.88972697	-0.99165683	0.61032188	1341.9247, 1353.5733, 1374.7930,
	H	0.51800441	-1.69018140	-0.14577229	1392.7745, 1408.0653, 1411.5426,
	H	1.46324133	-1.59435374	1.31938952	1414.1840, 1477.2795, 1485.1666,
	C	1.82235375	0.01608221	-0.05314579	1494.4202, 1500.8227, 1503.8851,
	H	1.28146411	0.57935406	-0.81614397	1504.5599, 1511.7220, 1513.8809,
	H	2.14070335	0.75287519	0.68902470	1731.8069, 3037.8914, 3042.2504,
	C	3.03817680	-0.65468412	-0.67864460	3052.7700, 3057.9999, 3058.5036,
	H	2.73401899	-1.37979524	-1.43550505	3065.1201, 3068.5875, 3070.3370,
	H	3.61922966	-1.18918120	0.07452804	3082.5100, 3095.1166, 3099.3505,
	H	3.69489181	0.07117994	-1.15660026	3120.6527, 3127.3542, 3131.7872,
	O	-0.04909478	2.79916229	-0.21944831	3136.1063, 3786.1600
	H	-0.84364772	3.30121250	0.02189701	
SP3_18	C	-2.96087823	-0.47235445	-0.27410513	598.2750i, 53.5430, 71.3843, 99.4230,
	H	-3.49912332	-0.19458965	0.63353506	109.0496, 123.7803, 160.9443,
	H	-3.66757291	-0.45469930	-1.10281228	211.2506, 240.0527, 274.6429,
	H	-2.61477121	-1.49937743	-0.15381461	326.9750, 337.9688, 390.3827,
	C	-0.84343242	0.56254167	0.65363448	433.4550, 527.6854, 669.7196,
	H	-0.05453215	1.35792609	0.37814731	727.3982, 760.7778, 806.6208,
	H	-1.34044228	1.01364579	1.51553424	833.1850, 880.3496, 889.4631,
	C	-1.79605742	0.48230364	-0.52746775	949.3138, 960.7852, 1002.5569,
	H	-1.25281194	0.17080540	-1.42200786	1033.9408, 1056.8114, 1068.3585,
	H	-2.17733597	1.48281630	-0.73431511	1097.7111, 1137.4362, 1164.3283,
	C	-0.17119727	-0.74047785	1.06165267	1178.3746, 1227.5838, 1253.7331,
	H	-0.92760980	-1.38729690	1.51619294	1292.9061, 1304.2290, 1332.7467,
	H	0.55100540	-0.53617357	1.85441408	1344.8823, 1369.4900, 1377.5581,
	C	0.50063229	-1.50625208	-0.07856326	1396.5910, 1404.2973, 1408.7441,
	H	-0.25960785	-1.83229437	-0.79216093	1414.3968, 1479.0548, 1489.8580,
	H	0.94683420	-2.41678074	0.32960556	1501.3251, 1502.6585, 1503.7376,
	C	1.57591630	-0.71645497	-0.82294348	1511.1958, 1513.7201, 1523.3310,
	H	1.96226520	-1.32977664	-1.63871275	1639.1298, 3045.0852, 3050.1867,
	H	1.12652221	0.16229272	-1.29151588	3054.2229, 3058.7156, 3061.8539,
	C	2.73666284	-0.29381865	0.07241545	3067.9719, 3077.5287, 3080.9067,
H	3.22633356	-1.16623921	0.50805884	3089.6168, 3097.4190, 3103.7125,	
H	2.40424472	0.32952190	0.90506437	3117.6770, 3123.5404, 3128.3112,	
H	3.48921573	0.26300869	-0.48667273	3135.4455, 3780.4198	
O	0.77727041	2.51416751	-0.05747027		
H	1.61934660	2.03094704	-0.06651595		
SP3_19	C	-2.20249682	1.95012316	-0.07941526	625.6510i, 46.2043, 67.8213, 69.3908,
	H	-3.13400086	1.39295042	-0.17991757	80.0951, 102.5913, 115.5365,
	H	-2.39267491	2.82737286	0.53739930	174.8296, 205.3475, 244.6676,
	H	-1.90953244	2.29456164	-1.07229463	256.7559, 291.8898, 302.6334,
	C	-0.83643934	-0.15704242	-0.32503168	430.2833, 506.9549, 654.6542,
	H	-1.84989051	-0.66533324	-0.50342715	724.3642, 744.9597, 796.1876,
	H	-0.51637030	0.12861789	-1.33048683	855.5710, 874.6040, 888.7598,
	C	-1.11966400	1.06609614	0.52534283	948.0973, 983.0378, 1046.1612,
	H	-0.19670162	1.64168237	0.64652636	1057.8998, 1066.5503, 1077.6322,
	H	-1.41687297	0.74124013	1.52611638	1122.7271, 1149.9682, 1178.6587,
	C	0.10226925	-1.17949875	0.29500573	1237.6864, 1249.5662, 1282.3530,
	H	0.22121699	-2.02077982	-0.39302563	1302.9301, 1315.5991, 1328.6533,
	H	-0.35748183	-1.57451336	1.20576624	1343.4385, 1374.3994, 1385.6314,
	C	1.48543700	-0.62474686	0.64466095	1405.2197, 1408.4868, 1413.2483,
	H	2.09273112	-1.43415636	1.05778598	1414.2308, 1482.0683, 1486.4600,
	H	1.39337755	0.12158949	1.43834515	1492.2525, 1499.3120, 1503.1012,
	C	2.21961687	-0.00806726	-0.54022610	1503.5606, 1510.3895, 1512.8221,
	H	2.24156168	-0.72733942	-1.36382638	1693.5590, 3036.5716, 3038.1711,
	H	1.66511821	0.85959248	-0.90544990	3043.5174, 3052.0680, 3057.7903,
	C	3.63874532	0.41309735	-0.18174077	3060.3073, 3063.2895, 3069.2178,
H	4.22613342	-0.44444829	0.14910995		

	H	3.63169578	1.14124379	0.63073961	3076.7024, 3087.7520, 3094.4089,
	H	4.15139569	0.86384445	-1.03062338	3123.9321, 3128.3369, 3132.8738,
	O	-3.11283734	-1.46096544	-0.31795555	3138.5885, 3782.9199
	H	-2.67181592	-2.21816974	0.09933267	
SP3_20	C	-2.56607230	-1.32531970	-0.48474309	542.6795i, 49.8416, 77.1927, 86.1381,
	H	-3.40498533	-1.04722005	0.15508684	113.3094, 115.6232, 172.9280,
	H	-2.96874012	-1.78274132	-1.38759170	181.8631, 213.9308, 256.2266,
	H	-1.98408539	-2.08240644	0.04163364	288.9200, 303.2821, 358.6908,
	C	-1.21295386	0.61150950	0.42203509	424.2052, 533.7593, 658.5946,
	H	-0.65468323	1.55421360	0.07455140	757.2114, 762.6711, 799.8468,
	H	-2.05015562	1.03098616	0.98466068	837.0289, 883.6498, 887.3303,
	C	-1.71460514	-0.10268974	-0.82175258	948.2870, 958.3202, 1029.1810,
	H	-0.86997191	-0.40384948	-1.44525071	1052.0911, 1063.0517, 1075.2547,
	H	-2.30014559	0.59906352	-1.41667436	1128.9586, 1155.3263, 1172.1773,
	C	-0.32330206	-0.20444627	1.35086294	1210.1095, 1253.3298, 1266.3196,
	H	-0.94980054	-0.92522075	1.88433009	1288.9656, 1294.4012, 1319.5296,
	H	0.08665003	0.45995773	2.11615965	1336.7577, 1356.6731, 1379.8144,
	C	0.81773054	-0.95574124	0.66868840	1391.0805, 1407.3152, 1408.6256,
	H	0.41338921	-1.69414405	-0.02981827	1413.6794, 1478.1630, 1485.5611,
	H	1.36382007	-1.52468429	1.42537878	1501.1596, 1501.6832, 1503.5308,
	C	1.80148503	-0.06008330	-0.07595446	1504.2991, 1512.9105, 1521.4329,
	H	1.28417456	0.46252015	-0.88448684	1625.7178, 3022.5528, 3041.5353,
H	2.17587858	0.70526340	0.61325730	3046.5193, 3058.0681, 3058.4705,	
C	2.97483096	-0.84318728	-0.65085856	3065.1891, 3068.3766, 3076.9314,	
H	2.62271095	-1.60455197	-1.34822028	3077.7335, 3090.8515, 3101.3615,	
H	3.52769150	-1.35027015	0.14085795	3124.5851, 3127.8041, 3134.1861,	
H	3.66896489	-0.19574505	-1.18507619	3135.1744, 3783.8895	
O	0.05484654	2.82399692	-0.26764179		
H	0.93783656	2.48660172	-0.04733007		
SP3_21	C	-3.12081987	-1.10874768	-0.28322204	484.4294i, 39.8561, 49.6384, 64.0362,
	H	-3.49689631	-0.11498320	-0.53014551	80.5491, 114.2852, 122.3188,
	H	-3.53567342	-1.81359178	-1.00249173	130.5216, 234.0029, 244.2449,
	H	-3.49753943	-1.37667453	0.70513031	263.3271, 290.6298, 313.6464,
	C	-1.00505721	-0.13763798	0.69231796	415.9267, 528.2113, 655.9780,
	H	-1.33213496	0.90735214	0.35755756	747.2621, 765.3257, 785.0517,
	H	-1.44982817	-0.28163043	1.68030457	854.2201, 880.8055, 905.6055,
	C	-1.59842592	-1.11559286	-0.30494954	946.7324, 966.5155, 1043.3464,
	H	-1.22219326	-2.11877518	-0.07785663	1046.7974, 1071.0972, 1091.7523,
	H	-1.24613787	-0.87113623	-1.30826431	1118.3095, 1159.4625, 1180.6049,
	C	0.51158226	-0.11069363	0.77501843	1209.7906, 1258.9587, 1283.1632,
	H	0.85699247	-1.08716251	1.12990642	1303.3086, 1304.4734, 1333.4611,
	H	0.81592324	0.61901795	1.53041279	1335.6018, 1370.0995, 1383.0010,
	C	1.18773822	0.23455464	-0.54971900	1399.4566, 1403.5325, 1410.8898,
	H	0.68237327	1.10260034	-0.98146679	1416.0111, 1478.1951, 1484.5973,
	H	1.05645465	-0.58946314	-1.25619556	1493.1978, 1497.8024, 1503.3844,
	C	2.67813936	0.53153736	-0.40752039	1506.2344, 1508.6630, 1512.3598,
	H	3.07610658	0.82193422	-1.38146426	1682.6622, 3032.5780, 3036.6809,
H	2.80884320	1.39530570	0.24957542	3045.3658, 3049.7433, 3057.0068,	
C	3.48015800	-0.64685059	0.13390027	3057.1382, 3065.2243, 3070.2339,	
H	3.32032624	-1.53645900	-0.47846187	3085.5093, 3092.5069, 3098.2717,	
H	3.19086899	-0.89133505	1.15596019	3123.8207, 3125.6026, 3132.9929,	
H	4.54787277	-0.43047781	0.13736073	3134.6001, 3781.1121	
O	-1.85715767	2.25553628	-0.10784289		
H	-2.51798569	2.34177272	0.59792762		
SP3_22	C	-2.57538429	-1.12261718	-0.87993029	610.2456i, 42.8651, 58.9654, 77.7712,
	H	-1.77005913	-1.54008834	-1.48390947	99.2896, 118.4891, 119.8995,
	H	-3.44289207	-1.77081542	-0.99573826	160.5323, 170.6703, 255.6795,
	H	-2.83312123	-0.14197446	-1.28367805	

	C	-1.03491133	-0.02739041	0.82877582	285.8497, 302.6152, 317.6851,
	H	-1.39438457	1.01429535	0.49699369	462.4401, 468.3082, 642.2027,
	H	-0.85021409	0.10074420	1.89841585	745.0106, 767.3442, 793.2932,
	C	-2.17415855	-1.00218961	0.58564327	852.0190, 878.5512, 908.7488,
	H	-3.03789189	-0.68911411	1.17373941	949.0260, 971.9529, 1019.2473,
	H	-1.87772849	-1.98437071	0.96801517	1032.8210, 1083.5364, 1104.1278,
	C	0.26314231	-0.32807907	0.10214435	1110.7450, 1155.4400, 1167.4976,
	H	0.10559301	-0.29181960	-0.98086123	1213.2617, 1254.1017, 1263.5150,
	H	0.55906551	-1.35743146	0.32993298	1298.4701, 1309.8957, 1325.7160,
	C	1.38114288	0.63842141	0.48027408	1361.4758, 1374.8496, 1380.1075,
	H	1.62271335	0.50465226	1.53921519	1402.8189, 1410.5662, 1415.8030,
	H	1.00807954	1.66074930	0.37739375	1417.4195, 1481.6247, 1483.3093,
	C	2.64995313	0.47266967	-0.35143955	1493.2402, 1500.1659, 1506.2307,
	H	2.41672883	0.66170242	-1.40294118	1506.8549, 1510.3340, 1512.5061,
	H	3.36942227	1.23778259	-0.05458810	1654.8944, 3028.7185, 3037.9826,
	C	3.29201062	-0.90331415	-0.21274920	3041.0572, 3048.4475, 3056.0481,
	H	2.64943324	-1.68752627	-0.61260440	3059.1639, 3061.8709, 3074.6040,
	H	3.48538959	-1.13471153	0.83640576	3085.4851, 3091.7062, 3092.5732,
	H	4.24052535	-0.95224952	-0.74623818	3125.5148, 3129.3450, 3134.4544,
	O	-1.72342516	2.25379124	-0.28464456	3136.1381, 3778.0428
	H	-1.27402653	1.97484148	-1.09870725	
	C	2.50365987	-1.18825023	0.88026486	
	H	1.69543945	-1.83512469	1.21974517	490.5791i, 30.9203, 54.3151, 62.4054,
	H	3.43849548	-1.73077835	1.01437784	78.3671, 88.9872, 112.0858, 147.3743,
	H	2.52473493	-0.30861807	1.52535748	162.5459, 259.1974, 273.9101,
	C	1.10653467	0.11905557	-0.79763004	314.0160, 324.3197, 459.0069,
	H	1.26612957	1.04395120	-0.14105374	463.9182, 648.6573, 743.6643,
	H	1.07900524	0.49059922	-1.82494596	772.8603, 778.4985, 843.0917,
	C	2.31675275	-0.77323332	-0.57481275	890.4628, 915.2183, 960.8070,
	H	3.20853495	-0.24766682	-0.91962043	977.3593, 1018.9469, 1032.2061,
	H	2.21682247	-1.66234820	-1.20581705	1081.1689, 1102.9017, 1109.6345,
	C	-0.23615876	-0.46826540	-0.40583621	1158.7475, 1188.3164, 1219.0002,
	H	-0.22394770	-0.71996415	0.65559082	1252.5474, 1261.7338, 1302.4871,
	H	-0.38491116	-1.40917066	-0.95036614	1317.0008, 1323.7770, 1361.5629,
	C	-1.39517152	0.47831846	-0.69657433	1368.5133, 1379.6433, 1384.5839,
	H	-1.34311383	0.79033901	-1.74338058	1407.3623, 1415.6996, 1419.1323,
	H	-1.26674699	1.38171705	-0.09199430	1478.7002, 1482.5238, 1492.7222,
	C	-2.77158739	-0.12178691	-0.42070782	1497.0894, 1505.1869, 1505.7096,
	H	-3.53598496	0.59849924	-0.71810524	1512.0427, 1512.9736, 1672.1929,
	H	-2.91343057	-1.00087405	-1.05509114	3017.0748, 3037.2339, 3038.1221,
	C	-2.98534805	-0.50644672	1.03927175	3047.7004, 3059.5905, 3062.6560,
	H	-2.78686273	0.34316251	1.69500960	3070.0315, 3074.3764, 3086.7822,
	H	-2.32496023	-1.31896894	1.34083652	3089.7153, 3105.4992, 3126.9942,
	H	-4.00959639	-0.83370951	1.21419257	3132.7346, 3135.5505, 3137.8725,
	O	1.38180058	2.28537738	0.72524009	3781.2416
	H	1.07389842	2.89958753	0.03949116	
SP3_23	C	2.50365987	-1.18825023	0.88026486	
	H	1.69543945	-1.83512469	1.21974517	
	H	3.43849548	-1.73077835	1.01437784	
	H	2.52473493	-0.30861807	1.52535748	
	C	1.10653467	0.11905557	-0.79763004	
	H	1.26612957	1.04395120	-0.14105374	
	H	1.07900524	0.49059922	-1.82494596	
	C	2.31675275	-0.77323332	-0.57481275	
	H	3.20853495	-0.24766682	-0.91962043	
	H	2.21682247	-1.66234820	-1.20581705	
	C	-0.23615876	-0.46826540	-0.40583621	
	H	-0.22394770	-0.71996415	0.65559082	
	H	-0.38491116	-1.40917066	-0.95036614	
	C	-1.39517152	0.47831846	-0.69657433	
	H	-1.34311383	0.79033901	-1.74338058	
	H	-1.26674699	1.38171705	-0.09199430	
	C	-2.77158739	-0.12178691	-0.42070782	
	H	-3.53598496	0.59849924	-0.71810524	
	H	-2.91343057	-1.00087405	-1.05509114	
	C	-2.98534805	-0.50644672	1.03927175	
	H	-2.78686273	0.34316251	1.69500960	
	H	-2.32496023	-1.31896894	1.34083652	
	H	-4.00959639	-0.83370951	1.21419257	
	O	1.38180058	2.28537738	0.72524009	
	H	1.07389842	2.89958753	0.03949116	
	C	3.22828244	-0.60444921	0.15492352	601.5596i, 35.1216, 66.3268, 82.5818,
	H	3.37729930	-0.95126704	-0.86873862	95.7964, 106.4653, 127.9601,
	H	4.18368309	-0.23709039	0.52746043	167.9570, 215.8416, 249.7995,
	H	2.94498753	-1.46343025	0.76143811	286.7372, 293.0537, 346.3886,
	C	0.84280976	0.07560021	-0.42048418	422.9649, 510.5868, 654.6433,
	H	0.15649992	0.99783294	-0.41940872	721.0588, 751.4629, 799.7535,
	H	0.96849921	-0.15925698	-1.48211847	849.3729, 853.9251, 913.6815,
	C	2.16556326	0.49093240	0.20409484	951.0794, 964.7447, 1012.6963,
	H	1.99237000	0.78884839	1.24169579	1045.1796, 1071.6171, 1084.8482,
	H	2.54494892	1.37235060	-0.31887961	1113.9632, 1147.7644, 1176.4437,
	C	0.10812798	-1.03990770	0.30014264	1181.8992, 1244.5375, 1270.0729,
	H	-0.09201576	-0.73006386	1.32940164	
SP3_24	C	3.22828244	-0.60444921	0.15492352	
	H	3.37729930	-0.95126704	-0.86873862	
	H	4.18368309	-0.23709039	0.52746043	
	H	2.94498753	-1.46343025	0.76143811	
	C	0.84280976	0.07560021	-0.42048418	
	H	0.15649992	0.99783294	-0.41940872	
	H	0.96849921	-0.15925698	-1.48211847	
	C	2.16556326	0.49093240	0.20409484	
	H	1.99237000	0.78884839	1.24169579	
	H	2.54494892	1.37235060	-0.31887961	
	C	0.10812798	-1.03990770	0.30014264	
	H	-0.09201576	-0.73006386	1.32940164	

	H	0.76993655	-1.90809082	0.36630922	1292.1155, 1318.9966, 1334.2072,
	C	-1.18630559	-1.47129092	-0.38774103	1365.3462, 1373.8060, 1378.1977,
	H	-1.61660320	-2.30587746	0.17206861	1391.3150, 1402.5704, 1408.8132,
	H	-0.94212321	-1.85751302	-1.38107413	1415.3998, 1478.6315, 1490.1937,
	C	-2.23962016	-0.37156503	-0.52006574	1491.1746, 1494.9537, 1502.5526,
	H	-1.86772579	0.42918853	-1.16221033	1507.0249, 1509.6397, 1514.9501,
	H	-3.11064809	-0.79169720	-1.02666412	1708.9676, 3040.2839, 3044.0031,
	C	-2.66524968	0.21574431	0.82038156	3045.3498, 3054.2679, 3055.6015,
	H	-1.84904313	0.76557799	1.28741136	3062.3984, 3063.1627, 3074.4600,
	H	-2.98619282	-0.57194013	1.50547588	3080.9779, 3088.0661, 3099.5480,
	H	-3.49306776	0.91273074	0.69607930	3125.7420, 3130.4460, 3139.4462,
	O	-0.37362962	2.39211770	-0.25764109	3139.7851, 3784.6138
	H	0.48658413	2.80237195	-0.07462734	
	C	3.05723639	-1.22369258	0.26108765	639.0892i, 43.7132, 57.3266, 62.3336,
	H	3.60639273	-0.28749641	0.36216364	94.5988, 108.8046, 121.2451,
	H	3.45213416	-1.93315328	0.98699614	134.5449, 229.4453, 244.1616,
	H	3.25166935	-1.62050822	-0.73635637	255.4934, 284.5943, 301.7761,
	C	0.99804226	-0.00355777	-0.53937292	414.2316, 529.0445, 644.1379,
	H	1.65944317	0.93326218	-0.48388473	742.6141, 755.8040, 787.9324,
	H	1.14257693	-0.36125295	-1.56336465	848.7330, 870.8717, 899.4232,
	C	1.56661867	-0.98702465	0.46586611	951.2291, 974.6337, 1039.1754,
	H	1.02677355	-1.93491796	0.38753051	1050.8444, 1076.5167, 1092.9466,
	H	1.38402901	-0.60634788	1.47454237	1117.8653, 1139.9147, 1184.6927,
	C	-0.44333347	0.41196006	-0.30467994	1227.9967, 1248.3125, 1290.4574,
	H	-0.71791253	1.19455554	-1.01828304	1298.8668, 1312.2679, 1330.4427,
	H	-0.52876163	0.84885757	0.69471442	1345.0461, 1378.3635, 1387.1646,
	C	-1.43081944	-0.74793929	-0.44046725	1393.3902, 1406.4642, 1412.6147,
	H	-1.27458847	-1.45647934	0.37719157	1416.2208, 1481.5935, 1485.0245,
	H	-1.21348325	-1.28782039	-1.36621488	1493.6823, 1499.8713, 1502.9320,
	C	-2.89162432	-0.30441949	-0.44484339	1506.0869, 1511.0746, 1513.2772,
	H	-3.06230024	0.35668059	-1.29853536	1701.1489, 3033.9823, 3041.8510,
	H	-3.52572288	-1.17916029	-0.60018004	3045.8353, 3049.5394, 3055.4202,
	C	-3.31276487	0.40196059	0.83896292	3058.5234, 3059.9062, 3068.3475,
	H	-2.78703299	1.34811268	0.96585547	3082.1252, 3085.7630, 3096.0490,
	H	-3.09598330	-0.21869046	1.71044082	3125.6241, 3127.9567, 3135.0427,
	H	-4.38057539	0.61719173	0.83857363	3138.4531, 3784.6220
	O	2.29170612	2.21479600	-0.01216765	
	H	1.46956146	2.58507769	0.34683272	
SP3_25	C	-3.34341613	-0.61943474	-0.14521651	481.6835i, 29.4102, 49.6756, 62.3579,
	H	-3.48164885	0.40491336	-0.49388682	75.9933, 91.3970, 110.1162, 127.0616,
	H	-3.94360086	-1.27364172	-0.77612673	228.5277, 243.3711, 262.7171,
	H	-3.73182561	-0.68504857	0.87230561	288.0665, 306.8422, 414.4050,
	C	-1.02033887	-0.08910916	0.68347136	519.6289, 653.6551, 736.9849,
	H	-1.09792294	0.96127254	0.23361784	763.8748, 781.8198, 855.7918,
	H	-1.45440776	-0.01093029	1.68356771	886.4030, 904.2547, 948.3794,
	C	-1.86858228	-0.99575118	-0.18943728	969.2020, 1037.0392, 1050.3487,
	H	-1.73293996	-2.03003180	0.14418916	1073.0418, 1091.0640, 1117.5736,
	H	-1.51260385	-0.95171272	-1.21956513	1154.9966, 1189.7467, 1208.7709,
	C	0.46165857	-0.41745864	0.76086585	1257.3349, 1281.1699, 1298.9137,
	H	0.58164405	-1.41496470	1.20032332	1312.2942, 1326.3168, 1340.6928,
	H	0.93577805	0.28371353	1.44933154	1373.3676, 1383.0654, 1399.2059,
	C	1.17206829	-0.37184658	-0.58844543	1408.4097, 1411.6633, 1417.0891,
	H	0.99605679	0.60735298	-1.04490455	1477.7529, 1485.0090, 1491.8184,
	H	0.72854574	-1.11259682	-1.25621141	1497.3473, 1504.1964, 1505.9132,
	C	2.67479519	-0.63016659	-0.49796688	1509.2351, 1513.0591, 1678.9879,
	H	2.84475242	-1.60682835	-0.03632562	3021.5127, 3037.0981, 3044.6458,
	H	3.08000552	-0.69455755	-1.50940939	3049.3381, 3057.3758, 3060.6956,
	C	3.43703545	0.44080011	0.27523433	
SP3_26	C	-3.34341613	-0.61943474	-0.14521651	481.6835i, 29.4102, 49.6756, 62.3579,
	H	-3.48164885	0.40491336	-0.49388682	75.9933, 91.3970, 110.1162, 127.0616,
	H	-3.94360086	-1.27364172	-0.77612673	228.5277, 243.3711, 262.7171,
	H	-3.73182561	-0.68504857	0.87230561	288.0665, 306.8422, 414.4050,
	C	-1.02033887	-0.08910916	0.68347136	519.6289, 653.6551, 736.9849,
	H	-1.09792294	0.96127254	0.23361784	763.8748, 781.8198, 855.7918,
	H	-1.45440776	-0.01093029	1.68356771	886.4030, 904.2547, 948.3794,
	C	-1.86858228	-0.99575118	-0.18943728	969.2020, 1037.0392, 1050.3487,
	H	-1.73293996	-2.03003180	0.14418916	1073.0418, 1091.0640, 1117.5736,
	H	-1.51260385	-0.95171272	-1.21956513	1154.9966, 1189.7467, 1208.7709,
	C	0.46165857	-0.41745864	0.76086585	1257.3349, 1281.1699, 1298.9137,
	H	0.58164405	-1.41496470	1.20032332	1312.2942, 1326.3168, 1340.6928,
	H	0.93577805	0.28371353	1.44933154	1373.3676, 1383.0654, 1399.2059,
	C	1.17206829	-0.37184658	-0.58844543	1408.4097, 1411.6633, 1417.0891,
	H	0.99605679	0.60735298	-1.04490455	1477.7529, 1485.0090, 1491.8184,
	H	0.72854574	-1.11259682	-1.25621141	1497.3473, 1504.1964, 1505.9132,
	C	2.67479519	-0.63016659	-0.49796688	1509.2351, 1513.0591, 1678.9879,
	H	2.84475242	-1.60682835	-0.03632562	3021.5127, 3037.0981, 3044.6458,
	H	3.08000552	-0.69455755	-1.50940939	3049.3381, 3057.3758, 3060.6956,
	C	3.43703545	0.44080011	0.27523433	

	H	3.15689079	0.45713187	1.32796403	3064.9709, 3084.4205, 3087.3883,
	H	3.23476061	1.43043739	-0.13787617	3096.4405, 3105.9698, 3126.9155,
	H	4.51196997	0.27006585	0.22613223	3127.6121, 3134.6725, 3136.6348,
	O	-1.29302902	2.34853171	-0.35317888	3779.8916
	H	-1.85054330	2.67497199	0.37127272	
SP3_27	C	2.68828136	-1.75508612	-0.06255939	474.9363i, 39.5419, 59.0360, 68.7598,
	H	2.82480460	-1.80334039	-1.14417404	89.5946, 114.2514, 131.1905,
	H	3.59742390	-2.12798121	0.40755832	144.7091, 178.3692, 251.8659,
	H	1.87594657	-2.43125580	0.20226938	292.4789, 307.1547, 324.6690,
	C	1.18848368	0.27304513	-0.32841809	461.0637, 468.4401, 630.2088,
	H	1.10096509	1.35585401	0.03940059	746.4768, 761.5871, 789.1063,
	H	1.37156899	0.35029740	-1.40432090	859.5561, 887.8222, 915.0903,
	C	2.39027511	-0.32478038	0.38298986	970.6399, 972.4386, 1018.1286,
	H	2.21319375	-0.30428400	1.46062489	1033.6583, 1079.6924, 1106.3972,
	H	3.26217897	0.30399021	0.19761360	1114.3894, 1157.0015, 1186.4531,
	C	-0.14203549	-0.40379256	-0.05786102	1223.4272, 1249.9848, 1269.1771,
	H	-0.26822338	-0.51755086	1.02176486	1299.8901, 1317.2193, 1318.9656,
	H	-0.12668190	-1.41493492	-0.47969175	1332.7621, 1363.9724, 1379.4484,
	C	-1.32197046	0.36211384	-0.64782451	1382.4707, 1403.8189, 1408.0745,
	H	-1.10557039	0.58762644	-1.69636520	1416.6211, 1480.6123, 1492.0209,
	H	-1.40967164	1.32209968	-0.13029047	1492.8568, 1499.3882, 1503.0827,
	C	-2.65094650	-0.38360094	-0.56015314	1507.5690, 1510.1389, 1513.2573,
	H	-3.42361547	0.21147864	-1.05039179	1668.4597, 3029.1735, 3039.1087,
	H	-2.57635273	-1.31725030	-1.12407463	3048.0868, 3053.3544, 3059.2185,
	C	-3.08059526	-0.68581284	0.87127757	3059.9540, 3063.0714, 3071.2718,
H	-3.10300493	0.22751859	1.46843617	3084.7048, 3093.2807, 3100.0891,	
H	-2.39612412	-1.38185597	1.35556535	3126.6651, 3129.1409, 3134.5596,	
H	-4.07511001	-1.12952399	0.89892296	3137.5941, 3782.9787	
O	0.91365950	2.81578248	0.35985194		
H	0.50004213	3.05033582	-0.48637056		
SP3_28	C	-2.33028452	-2.07675697	0.09061698	465.9186i, 33.7786, 57.7526, 63.8302,
	H	-2.28974424	-2.21307785	1.17257093	78.2611, 101.8927, 111.3111,
	H	-3.22664223	-2.57486518	-0.27691054	146.2286, 164.4966, 250.8306,
	H	-1.46824336	-2.58305848	-0.34250219	271.9255, 309.8427, 331.9304,
	C	-1.16535947	0.16749844	0.31502161	458.0024, 463.7624, 627.1961,
	H	-1.32384224	1.26996885	0.04638048	743.5881, 774.4256, 783.8551,
	H	-1.18120777	0.12931799	1.40863064	870.6951, 883.9494, 913.7139,
	C	-2.34467421	-0.59230168	-0.26859651	964.6451, 980.0841, 1016.9073,
	H	-2.34096284	-0.47572289	-1.35464349	1034.9820, 1080.6034, 1103.7391,
	H	-3.27053117	-0.14028511	0.08998045	1109.1602, 1154.9035, 1192.0455,
	C	0.20085213	-0.22610770	-0.21424932	1208.8346, 1247.7779, 1275.2918,
	H	0.18932710	-0.18418090	-1.30826976	1294.3357, 1323.3685, 1328.4371,
	H	0.39825661	-1.26694001	0.05676216	1334.9240, 1362.7134, 1378.6203,
	C	1.31803382	0.66478852	0.31821815	1385.1544, 1402.0973, 1409.8708,
	H	1.35998539	0.57094530	1.40856158	1415.1240, 1478.5844, 1491.6067,
	H	1.06324583	1.70474187	0.10037771	1492.4931, 1497.9235, 1502.1552,
	C	2.69267398	0.34970822	-0.26595863	1506.0632, 1510.3421, 1512.1418,
	H	2.65802286	0.48310256	-1.35031280	1679.2057, 3030.3877, 3039.2013,
	H	3.41126010	1.08007598	0.11035837	3051.3638, 3052.9138, 3058.1745,
	C	3.18775458	-1.05521501	0.05986631	3060.0183, 3063.5156, 3072.7969,
H	2.56488743	-1.81853606	-0.40588300	3086.6824, 3093.8750, 3099.5083,	
H	3.17641115	-1.22861165	1.13767149	3124.9682, 3129.1012, 3134.9655,	
H	4.20782528	-1.20522028	-0.29193809	3137.2787, 3781.6594	
O	-1.50147133	2.75743187	-0.14670654		
H	-1.27025519	3.00320788	0.76330680		
SP3_29	C	-3.10803955	-1.16750725	0.16427405	461.3798i, 28.1822, 47.2869, 60.6516,
	H	-3.64745073	-0.27999120	-0.16804449	67.1000, 85.8776, 110.4406, 129.2257,
	H	-3.61408586	-2.04309887	-0.24006396	232.2545, 248.0555, 277.7176,

	H	-3.17449449	-1.21625551	1.25262054	288.5167, 297.8032, 416.8327,
	C	-0.92177712	0.09271793	0.29529824	527.5478, 623.7893, 734.4732,
	H	-1.52626823	1.02222230	0.00819013	769.1375, 786.2042, 869.2778,
	H	-0.94062613	0.06347231	1.38912818	883.0879, 909.2305, 951.5852,
	C	-1.65394444	-1.10345957	-0.28495970	966.5956, 1042.6011, 1052.2133,
	H	-1.13885585	-2.02050550	0.01344075	1075.6964, 1089.4101, 1115.5587,
	H	-1.60185455	-1.05733752	-1.37551537	1152.3657, 1190.9410, 1223.8582,
	C	0.49055243	0.32326728	-0.21458029	1234.2479, 1291.7489, 1299.1543,
	H	0.83920426	1.29184834	0.14657254	1309.3900, 1328.3946, 1339.7983,
	H	0.47429010	0.38309932	-1.30703558	1345.4413, 1378.9803, 1392.1334,
	C	1.47091174	-0.76795413	0.21573530	1399.7539, 1410.0247, 1416.3215,
	H	1.10824854	-1.73741352	-0.13105836	1480.6686, 1486.8784, 1491.9387,
	H	1.49391199	-0.81585479	1.30939459	1500.2199, 1502.9601, 1505.1537,
	C	2.88928814	-0.55507421	-0.30984630	1510.4370, 1513.3061, 1694.3808,
	H	3.49759814	-1.41894241	-0.03521061	3034.9934, 3045.8173, 3047.0791,
	H	2.86496396	-0.53041702	-1.40243213	3051.5510, 3056.8045, 3057.5742,
	C	3.55436779	0.71257171	0.21490694	3060.1735, 3080.4710, 3087.0519,
	H	3.53719004	0.73393626	1.30618719	3089.1378, 3107.5309, 3124.5039,
	H	3.05124129	1.60992946	-0.14333900	3126.8202, 3135.9715, 3137.8202,
	H	4.59446689	0.77080019	-0.10384004	3784.2202
	O	-2.41183483	2.23112460	-0.20760657	
	H	-2.85095473	2.18814077	0.65688875	
	C	-2.05545979	-1.40363684	-0.85281755	
	H	-1.12961803	-1.59032501	-1.39834410	600.3718i, 28.4723, 40.7076, 54.7592,
	H	-2.68127042	-2.28907418	-0.95444552	78.7183, 84.5202, 125.2500, 170.7146,
	H	-2.56851516	-0.56816371	-1.33186323	219.8626, 249.1675, 285.8529,
	C	-1.04149468	0.22128714	0.82184674	296.4108, 340.7662, 435.8465,
	H	-1.75948314	1.05866567	0.50537175	513.4398, 649.6787, 727.5013,
	H	-0.87385199	0.40856669	1.88513609	754.3454, 799.0910, 850.1016,
	C	-1.78695878	-1.08814229	0.61341836	856.0005, 902.1214, 957.6677,
	H	-2.73223683	-1.03697618	1.15560256	966.2098, 1012.2011, 1043.7804,
	H	-1.21806486	-1.90272187	1.07107259	1072.7236, 1097.4202, 1122.9562,
	C	0.25172230	0.39271515	0.04021486	1141.9540, 1166.7422, 1225.5203,
	H	0.66127570	1.38038989	0.26031406	1243.7510, 1286.5424, 1293.4924,
	H	0.04429977	0.37176180	-1.03453930	1318.6055, 1332.3563, 1363.1718,
	C	1.29188534	-0.67925734	0.36082847	1375.3466, 1378.4886, 1396.7145,
	H	0.87171745	-1.66253356	0.13776447	1401.0844, 1413.9477, 1415.9346,
	H	1.49871727	-0.66677129	1.43591638	1481.0770, 1490.0226, 1491.9512,
	C	2.60006963	-0.51372599	-0.40963948	1496.7506, 1503.7681, 1507.0698,
	H	3.24034601	-1.37292151	-0.20168990	1512.7149, 1515.8449, 1690.7656,
	H	2.38850308	-0.54052806	-1.48203640	3033.2804, 3043.7385, 3046.7087,
	C	3.35577332	0.76603923	-0.06909354	3049.5708, 3059.2635, 3060.8055,
	H	3.52964175	0.83662711	1.00614520	3072.7965, 3082.2011, 3087.0065,
	H	2.80502312	1.65471517	-0.37553627	3090.9273, 3100.9642, 3125.9956,
	H	4.32448587	0.79415034	-0.56656841	3127.8453, 3135.7731, 3137.2933,
	O	-2.53311125	2.08774330	-0.27699077	3783.9085
	H	-1.82930368	2.25151791	-0.92492097	
	C	-3.17410692	-1.11342333	0.16224349	
	H	-3.68687344	-0.15879939	0.04393942	643.2775i, 26.1053, 56.7273, 65.1062,
	H	-3.72541386	-1.87046836	-0.39380083	84.8728, 100.8535, 120.9810,
	H	-3.20663376	-1.38284765	1.21888134	128.1729, 218.1147, 247.6615,
	C	-0.95065998	0.04603757	0.44344770	257.5613, 285.2078, 293.1566,
	H	-1.56583966	1.01349211	0.38364568	416.5186, 519.2477, 642.0684,
	H	-0.93328501	-0.17946043	1.51416897	733.5532, 754.1535, 787.5508,
	C	-1.73398422	-1.00381490	-0.32192914	857.2050, 870.2352, 899.9284,
	H	-1.23704116	-1.97263601	-0.22294595	951.3111, 974.5694, 1043.7365,
	H	-1.71668301	-0.75162876	-1.38573605	1046.5780, 1076.3744, 1090.5852,
	C	0.44728898	0.34019879	-0.07286794	1116.9195, 1140.3273, 1183.8911,
SP3_30					
SP3_31					

	H	0.83929530	1.21545293	0.44883602	1231.6673, 1241.7376, 1287.7462,
	H	0.39393139	0.60058543	-1.13622813	1302.6059, 1308.5772, 1337.8955,
	C	1.41452063	-0.83034308	0.10020791	1343.7940, 1376.7734, 1389.0081,
	H	1.01193660	-1.70804080	-0.40854637	1395.4521, 1404.8411, 1413.0143,
	H	1.47552135	-1.08581879	1.16296836	1416.6076, 1481.4199, 1485.0968,
	C	2.81794625	-0.54951802	-0.43323989	1492.2808, 1500.3486, 1503.6651,
	H	3.41098316	-1.46249077	-0.35454528	1505.3166, 1511.8136, 1512.8015,
	H	2.75489067	-0.31489445	-1.49916762	1708.3503, 3025.6744, 3041.7191,
	C	3.53811601	0.57876279	0.29691657	3044.5006, 3051.4147, 3057.3141,
	H	3.56075635	0.39019799	1.37177904	3059.9120, 3060.4417, 3077.1859,
	H	3.04940323	1.53953377	0.13856744	3085.4469, 3089.0937, 3102.5881,
	H	4.56724556	0.67488790	-0.04708061	3126.8781, 3128.8280, 3137.0190,
	O	-2.20806482	2.26990490	-0.14181520	3138.2398, 3784.3378
	H	-1.48239973	2.48629721	-0.74888607	
	C	-3.81332056	-0.62861386	-0.19201950	
	H	-3.88108854	-1.67688837	0.10278541	477.8041i, 21.7177, 61.3957, 64.5163,
	H	-4.70086522	-0.11807318	0.17977802	68.4984, 83.7073, 97.3367, 146.4046,
	H	-3.83658006	-0.58950650	-1.28187326	168.0912, 245.2546, 248.5630,
	C	-1.28115278	-0.69312682	-0.16547883	249.0780, 307.0389, 415.5852,
	H	-1.30647842	-1.74963742	0.12544126	490.8711, 617.4731, 735.0756,
	H	-1.27192860	-0.67580110	-1.25915706	752.4520, 822.3048, 846.8772,
	C	-2.53612651	0.00500137	0.34295261	896.8797, 926.9142, 950.2160,
	H	-2.49212268	1.05781349	0.05474213	1022.5616, 1024.8165, 1066.0965,
	H	-2.54128993	-0.01967499	1.43602946	1090.8080, 1091.7504, 1096.4144,
	C	0.00016124	-0.07187517	0.35366978	1169.9944, 1202.9729, 1211.1238,
	H	0.00018203	-0.02992163	1.44709757	1248.2211, 1278.0476, 1283.3965,
	H	0.00004906	1.02101848	0.00869194	1309.6159, 1326.7099, 1336.2212,
	C	1.28158432	-0.69285143	-0.16554803	1359.9826, 1366.3082, 1402.1338,
	H	1.27240482	-0.67531528	-1.25922303	1405.2085, 1413.5688, 1414.1004,
	H	1.30702168	-1.74941837	0.12516111	1477.8022, 1486.1682, 1497.6686,
	C	2.53645348	0.00531905	0.34308143	1498.3248, 1503.3221, 1503.3963,
	H	2.49230268	1.05822119	0.05522284	1512.1922, 1512.9538, 1676.2909,
	H	2.54164150	-0.01969979	1.43614771	3023.1779, 3027.6958, 3048.4332,
	C	3.81373589	-0.62792649	-0.19211744	3049.1351, 3051.6255, 3057.2203,
	H	3.83699313	-0.58843110	-1.28195704	3057.5706, 3065.3347, 3073.9752,
	H	3.88164619	-1.67629608	0.10231769	3090.0601, 3092.3587, 3124.0581,
	H	4.70120787	-0.11739536	0.17986618	3124.2128, 3132.8206, 3132.9152,
	O	-0.00108820	2.49571177	-0.33748997	3784.9289
	H	-0.00240035	2.80775191	0.58160866	
SP4_1	C	-3.81139355	-0.54566225	-0.24622799	
	H	-3.87923287	-1.63413191	-0.21423559	654.3588i, 60.7279, 61.7822, 62.9867,
	H	-4.70045742	-0.14044124	0.23521922	77.9287, 81.1383, 101.7059, 153.5370,
	H	-3.83241503	-0.24433498	-1.29460150	155.8558, 244.7787, 246.8357,
	C	-1.27945403	-0.61631481	-0.22463198	250.3963, 307.0031, 421.3146,
	H	-1.30335535	-1.71152376	-0.19307596	491.1176, 612.8521, 733.8984,
	H	-1.27160694	-0.34620419	-1.28627532	753.9775, 817.0015, 846.4811,
	C	-2.53710972	-0.05983863	0.43115117	896.4326, 926.2514, 931.0890,
	H	-2.49238114	1.03133424	0.40944855	1020.8695, 1021.9852, 1065.9560,
	H	-2.54566289	-0.34762967	1.48541120	1089.8239, 1090.0924, 1096.7922,
	C	0.00060799	-0.13252284	0.42618549	1165.6269, 1182.6058, 1214.9691,
	H	0.00055876	-0.34222585	1.50020046	1245.6010, 1274.5219, 1278.8265,
	H	0.00159836	1.01766898	0.38584169	1311.6070, 1326.4025, 1335.8372,
	C	1.28047519	-0.61611846	-0.22502560	1367.5111, 1401.6930, 1405.1097,
	H	1.27226464	-0.34516978	-1.28634742	1407.8670, 1413.5587, 1414.1550,
	H	1.30467505	-1.71135027	-0.19355904	1478.7572, 1487.2728, 1497.5589,
	C	2.53788303	-0.05897831	0.43058045	1498.0698, 1503.7517, 1503.8320,
	H	2.49236230	1.03208589	0.40799481	1512.4799, 1512.9333, 1697.5813,
	H	2.54677586	-0.34649621	1.48493644	3020.6955, 3024.5587, 3047.4966,
SP4_2	C	-3.81139355	-0.54566225	-0.24622799	
	H	-3.87923287	-1.63413191	-0.21423559	654.3588i, 60.7279, 61.7822, 62.9867,
	H	-4.70045742	-0.14044124	0.23521922	77.9287, 81.1383, 101.7059, 153.5370,
	H	-3.83241503	-0.24433498	-1.29460150	155.8558, 244.7787, 246.8357,
	C	-1.27945403	-0.61631481	-0.22463198	250.3963, 307.0031, 421.3146,
	H	-1.30335535	-1.71152376	-0.19307596	491.1176, 612.8521, 733.8984,
	H	-1.27160694	-0.34620419	-1.28627532	753.9775, 817.0015, 846.4811,
	C	-2.53710972	-0.05983863	0.43115117	896.4326, 926.2514, 931.0890,
	H	-2.49238114	1.03133424	0.40944855	1020.8695, 1021.9852, 1065.9560,
	H	-2.54566289	-0.34762967	1.48541120	1089.8239, 1090.0924, 1096.7922,
	C	0.00060799	-0.13252284	0.42618549	1165.6269, 1182.6058, 1214.9691,
	H	0.00055876	-0.34222585	1.50020046	1245.6010, 1274.5219, 1278.8265,
	H	0.00159836	1.01766898	0.38584169	1311.6070, 1326.4025, 1335.8372,
	C	1.28047519	-0.61611846	-0.22502560	1367.5111, 1401.6930, 1405.1097,
	H	1.27226464	-0.34516978	-1.28634742	1407.8670, 1413.5587, 1414.1550,
	H	1.30467505	-1.71135027	-0.19355904	1478.7572, 1487.2728, 1497.5589,
	C	2.53788303	-0.05897831	0.43058045	1498.0698, 1503.7517, 1503.8320,
	H	2.49236230	1.03208589	0.40799481	1512.4799, 1512.9333, 1697.5813,
	H	2.54677586	-0.34649621	1.48493644	3020.6955, 3024.5587, 3047.4966,

	C	3.81227417	-0.54437556	-0.24689085	3049.9607, 3053.4054, 3054.5655,
	H	3.83289788	-0.24309907	-1.29527347	3057.7672, 3058.0743, 3068.1973,
	H	3.88069938	-1.63281756	-0.21474471	3091.2772, 3092.3346, 3123.5916,
	H	4.70121898	-0.13861532	0.23433708	3123.7492, 3133.2117, 3133.3356,
	O	0.00122757	2.42273615	-0.14459281	3781.2950
	H	-0.03745875	2.16392672	-1.07937815	
SP4_3	C	-3.11897880	0.48263925	0.28091154	702.7703i, 54.1792, 73.5841, 90.6933,
	H	-3.14580304	0.98224555	-0.69150704	115.8662, 126.8158, 134.7544,
	H	-4.13141164	0.49909117	0.68223371	154.8231, 186.3707, 250.1135,
	H	-2.49031148	1.06764878	0.95317400	271.7384, 318.3808, 361.4882,
	C	-1.22534613	-1.03639598	-0.51306243	394.0430, 494.8499, 645.7859,
	H	-0.95938155	-2.09104734	-0.63515069	707.6138, 757.4931, 777.3368,
	H	-1.26085015	-0.61336428	-1.52221344	849.6010, 885.1481, 921.4972,
	C	-2.60401357	-0.94475539	0.13546638	928.8622, 986.3991, 1035.3957,
	H	-2.56547599	-1.41688546	1.12036426	1062.9473, 1084.9246, 1097.0933,
	H	-3.31352385	-1.52456133	-0.45725063	1113.5874, 1149.3399, 1180.8218,
	C	-0.11537387	-0.35699304	0.26733850	1224.8670, 1255.1116, 1272.4610,
	H	-0.18917619	-0.57277682	1.33827202	1289.5101, 1307.9656, 1332.8294,
	H	-0.24012655	0.78551214	0.20038207	1345.7594, 1369.9467, 1378.8153,
	C	1.27960923	-0.63093974	-0.25759539	1396.7000, 1408.4750, 1411.9378,
	H	1.31821137	-0.36304490	-1.31771206	1415.7391, 1475.4023, 1484.6809,
	H	1.47653060	-1.70774887	-0.20139756	1495.9916, 1497.3204, 1504.8495,
	C	2.36408876	0.12743171	0.49674210	1507.9074, 1511.9120, 1520.8257,
	H	2.14946285	1.19629647	0.43808630	1661.2202, 3024.0145, 3032.4272,
H	2.31925735	-0.14259793	1.55510944	3042.8812, 3048.9593, 3051.3312,	
C	3.75710904	-0.15611532	-0.04901179	3053.3704, 3056.4934, 3068.0788,	
H	3.82674532	0.13304264	-1.09854054	3074.8640, 3091.0072, 3095.8480,	
H	3.99360701	-1.21925424	0.01781262	3116.3047, 3124.2936, 3131.4989,	
H	4.52176762	0.39211114	0.49997316	3133.9270, 3784.5498	
O	-0.26580912	2.18999331	-0.31163601		
H	-1.20561670	2.16615781	-0.55328101		
SP4_4	C	3.30671244	-0.56626079	0.64874521	490.2542i, 56.7728, 70.8431, 77.4543,
	H	3.50597020	-1.56040714	0.24602841	90.5940, 106.6770, 148.9495,
	H	4.24155065	-0.00717399	0.63871353	153.9416, 212.7131, 247.4027,
	H	2.99906814	-0.68585206	1.68834127	283.1898, 299.8317, 380.8855,
	C	0.90488970	-0.62595342	-0.15625104	403.0925, 482.5238, 641.9337,
	H	1.06275032	-1.63082424	-0.56655591	742.6487, 775.6690, 815.2912,
	H	0.57256356	-0.76534891	0.87583909	848.9820, 860.4989, 919.9575,
	C	2.22284616	0.13793300	-0.15655713	953.7924, 976.1206, 1032.8874,
	H	2.04788651	1.13636973	0.25204457	1038.8886, 1073.5180, 1092.7990,
	H	2.55878432	0.27441915	-1.18805109	1118.1165, 1162.3312, 1178.0841,
	C	-0.18142940	0.06510912	-0.95798958	1203.6931, 1252.2358, 1265.5542,
	H	0.18994954	0.33666284	-1.94933110	1290.5838, 1295.3173, 1309.9513,
	H	-0.39624318	1.06855859	-0.44298671	1334.4577, 1361.2450, 1374.6651,
	C	-1.49981539	-0.68524232	-1.07722481	1390.3927, 1407.2746, 1414.0536,
	H	-1.33641885	-1.56106846	-1.71370347	1420.5616, 1475.1580, 1481.5787,
	H	-2.21963650	-0.05117800	-1.60058374	1495.5994, 1497.7448, 1503.4090,
	C	-2.10203503	-1.13498996	0.25264262	1505.3030, 1511.1520, 1513.3625,
	H	-3.04202241	-1.65045044	0.04779786	1725.6635, 3020.8277, 3034.0844,
H	-1.44795512	-1.87352584	0.72142101	3046.3013, 3057.0125, 3057.4795,	
C	-2.35170738	0.01933183	1.21657486	3061.9447, 3065.9297, 3074.6027,	
H	-2.96091232	0.79244412	0.74573033	3077.0993, 3090.2343, 3094.8124,	
H	-1.42057734	0.49320006	1.52757432	3124.0103, 3129.2792, 3133.2127,	
H	-2.86932710	-0.32293061	2.11193771	3136.8024, 3783.5074	
O	-0.43135334	2.48613377	0.07244333		
H	0.16862978	2.85847028	-0.59340358		
SP4_5	C	-3.42371453	-0.98685344	-0.51678907	486.4546i, 50.2432, 52.0972, 62.4641,
	H	-3.42300197	-1.98817608	-0.08359055	67.9615, 98.7531, 101.3189, 138.1186,

	H	-4.43911099	-0.59689897	-0.45711498	205.3233, 239.6157, 245.5886,
	H	-3.16299938	-1.08243871	-1.57158479	278.1723, 311.0616, 405.3714,
	C	-1.00408193	-0.60958293	0.13373481	506.8354, 656.3427, 738.0813,
	H	-0.95773055	-1.60899805	0.58297322	742.8796, 812.1865, 853.4574,
	H	-0.71871624	-0.72776089	-0.91422896	869.4497, 919.2031, 949.8407,
	C	-2.43193555	-0.08346032	0.20376477	992.9400, 1031.6279, 1060.9229,
	H	-2.45655971	0.91767108	-0.23405395	1073.5778, 1093.4989, 1111.9837,
	H	-2.72421662	0.02507021	1.25165396	1163.3962, 1192.2529, 1217.0358,
	C	-0.00850257	0.29301619	0.83762355	1267.5457, 1275.5299, 1284.3830,
	H	-0.36163072	0.54351911	1.84108927	1317.1583, 1330.3269, 1333.9607,
	H	0.00084215	1.28154115	0.26000998	1364.9040, 1383.5297, 1402.0773,
	C	1.42917614	-0.19649669	0.87433600	1405.9363, 1413.3329, 1414.3995,
	H	1.47248769	-1.12924320	1.44861934	1478.7826, 1480.5069, 1495.8169,
	H	2.03847649	0.52889123	1.41913962	1497.1204, 1503.7998, 1503.9932,
	C	2.04281778	-0.42186319	-0.50349321	1510.6067, 1511.6929, 1675.2015,
	H	1.51141612	-1.22498726	-1.01732857	3020.8203, 3024.5703, 3045.9866,
	H	1.90133813	0.48097009	-1.10316900	3054.5933, 3057.3706, 3057.9659,
	C	3.52378447	-0.76747072	-0.42031728	3063.8924, 3072.6003, 3075.5740,
	H	3.67944092	-1.66932568	0.17401397	3091.0921, 3098.0254, 3123.7796,
	H	4.08427494	0.04043514	0.05191148	3124.1141, 3132.3628, 3133.5735,
	H	3.95130322	-0.93949546	-1.40734340	3779.8407
	O	-0.07348081	2.58992565	-0.50853090	
	H	-0.57302985	3.06608771	0.17409326	
	C	-3.43177915	-0.86864328	-0.58894792	608.7781i, 57.0744, 64.1779, 71.1127,
	H	-3.41418517	-1.92826063	-0.32964446	88.2891, 101.8189, 140.6647,
	H	-4.45075595	-0.50800765	-0.45462368	157.4851, 202.5031, 239.4301,
	H	-3.18432207	-0.78432442	-1.64822946	249.9033, 261.7343, 310.4889,
	C	-1.01026368	-0.57694393	0.09872922	406.3624, 516.9392, 644.2392,
	H	-0.94849629	-1.63159218	0.39242624	738.9674, 749.7197, 817.9866,
	H	-0.73860527	-0.54474798	-0.96079508	851.6579, 868.6898, 917.5883,
	C	-2.44306509	-0.08456029	0.26326227	937.9480, 988.8229, 1031.3251,
	H	-2.48433044	0.97677380	0.00645570	1059.6510, 1073.2099, 1094.1436,
	H	-2.72465718	-0.15571809	1.31671933	1111.1302, 1162.3279, 1174.9779,
	C	-0.01296718	0.22175373	0.91729162	1214.8266, 1270.7418, 1271.7795,
	H	-0.36539068	0.32886503	1.94627849	1281.7507, 1317.8937, 1329.2849,
	H	-0.02079324	1.30398609	0.52564971	1331.8010, 1367.2881, 1398.5516,
	C	1.42269117	-0.27121867	0.88441835	1407.0237, 1413.2260, 1414.1522,
	H	1.45979850	-1.27383091	1.32634863	1418.0697, 1479.6462, 1484.8272,
	H	2.03502039	0.36932685	1.52343044	1496.1108, 1498.1234, 1504.1898,
	C	2.04304286	-0.31723806	-0.50786303	1504.3857, 1510.3243, 1513.3969,
	H	1.49164812	-1.01901009	-1.13673117	1651.2877, 3021.3768, 3024.8076,
	H	1.94443270	0.66925391	-0.96944386	3049.2240, 3051.9997, 3056.3957,
	C	3.51125875	-0.72093035	-0.46735316	3058.1375, 3058.8078, 3073.0192,
	H	3.62960655	-1.70626363	-0.01413246	3076.3436, 3089.8214, 3095.1594,
	H	4.09085664	-0.01223051	0.12537219	3123.1635, 3125.4284, 3133.7529,
	H	3.94534760	-0.75733265	-1.46573627	3134.5930, 3778.8678
	O	-0.07170364	2.53887286	-0.32625696	
	H	-0.16505116	2.06881538	-1.17051275	
SP4_6	C	3.32978492	-0.45949652	0.68209176	553.9667i, 51.9132, 69.6885, 76.1345,
	H	3.53509503	-1.48447187	0.36914900	123.1812, 131.6262, 154.7402,
	H	4.26366708	0.09901757	0.63229747	172.7710, 222.3045, 248.8406,
	H	3.01352890	-0.48952772	1.72574041	281.4193, 321.8434, 377.2870,
	C	0.93891863	-0.59797940	-0.14215736	401.7064, 507.6379, 665.2807,
	H	1.09850500	-1.62714751	-0.48717487	735.6475, 764.8637, 799.6833,
	H	0.60741044	-0.67367138	0.89739062	845.8847, 860.6661, 920.4363,
	C	2.25340882	0.17074187	-0.19121642	944.4145, 966.8930, 1033.7318,
	H	2.06861572	1.19989447	0.12448853	1047.0130, 1073.7675, 1096.2988,
	H	2.59928514	0.22158447	-1.22664472	
SP4_7	C	3.32978492	-0.45949652	0.68209176	553.9667i, 51.9132, 69.6885, 76.1345,
	H	3.53509503	-1.48447187	0.36914900	123.1812, 131.6262, 154.7402,
	H	4.26366708	0.09901757	0.63229747	172.7710, 222.3045, 248.8406,
	H	3.01352890	-0.48952772	1.72574041	281.4193, 321.8434, 377.2870,
	C	0.93891863	-0.59797940	-0.14215736	401.7064, 507.6379, 665.2807,
	H	1.09850500	-1.62714751	-0.48717487	735.6475, 764.8637, 799.6833,
	H	0.60741044	-0.67367138	0.89739062	845.8847, 860.6661, 920.4363,
	C	2.25340882	0.17074187	-0.19121642	944.4145, 966.8930, 1033.7318,
	H	2.06861572	1.19989447	0.12448853	1047.0130, 1073.7675, 1096.2988,
	H	2.59928514	0.22158447	-1.22664472	

	C	-0.14573950	0.04198382	-0.98667165	1124.3649, 1163.9933, 1170.9712,
	H	0.22775337	0.25935872	-1.99006800	1219.6770, 1239.0058, 1274.4634,
	H	-0.31754794	1.09662059	-0.56059599	1279.9491, 1290.4648, 1309.1204,
	C	-1.46157153	-0.71647730	-1.07201851	1334.9288, 1364.5047, 1377.9713,
	H	-1.30129833	-1.59911992	-1.69916311	1392.2426, 1408.6428, 1411.5324,
	H	-2.19497782	-0.09847356	-1.59710191	1413.1511, 1475.8555, 1482.0313,
	C	-2.04619140	-1.16708214	0.26552334	1496.2193, 1502.3212, 1503.5838,
	H	-2.97187999	-1.71153453	0.07208200	1506.8290, 1511.2124, 1522.1793,
	H	-1.36849050	-1.87894133	0.74101345	1636.7208, 3018.0803, 3036.0252,
	C	-2.32794998	-0.01663243	1.22458003	3043.7315, 3052.2785, 3056.6004,
	H	-2.98033690	0.72440071	0.75450279	3059.7994, 3066.1092, 3074.9757,
	H	-1.40662803	0.48113617	1.53050318	3080.1414, 3092.8325, 3095.0197,
	H	-2.82805027	-0.36638408	2.12674530	3116.3878, 3123.3752, 3132.6881,
	O	-0.48816054	2.49646360	-0.04860397	3133.3905, 3782.3060
	H	-1.38332622	2.34520312	0.29488042	
	C	-3.73369767	-0.63663217	-0.17975478	468.0661i, 54.8086, 61.8200, 66.2552,
	H	-3.79706876	-0.54468201	-1.26484598	71.5692, 94.6934, 126.8196, 147.8879,
	H	-4.29569150	-1.52209661	0.11517334	212.4304, 244.4813, 248.3003,
	H	-4.22546987	0.23456727	0.25478814	284.2087, 310.3108, 404.8203,
	C	-1.47991265	0.51184358	-0.15225691	512.3059, 622.3684, 739.7578,
	H	-1.46359458	0.57306473	-1.24412328	745.1235, 818.9144, 854.8745,
	H	-1.99421238	1.40861378	0.20123066	883.7699, 918.5554, 954.8542,
	C	-2.28084031	-0.71911183	0.27034308	989.8860, 1045.3597, 1057.2924,
	H	-2.23409653	-0.82149852	1.35798141	1074.5188, 1090.0918, 1110.9645,
	H	-1.82045785	-1.61700570	-0.14604827	1161.4101, 1193.4742, 1219.4882,
	C	-0.05442965	0.51418931	0.37116032	1249.5221, 1286.1135, 1295.2236,
	H	-0.04130158	0.53889972	1.46493878	1320.2500, 1326.3249, 1331.0923,
	H	0.41012979	1.50811481	0.04056613	1339.4903, 1373.5149, 1392.6034,
	C	0.84292084	-0.59207694	-0.15034790	1403.5967, 1412.2398, 1413.6659,
	H	0.78518028	-0.61879403	-1.24286343	1481.3504, 1486.0082, 1497.1006,
	H	0.46920012	-1.55855095	0.20380014	1497.9120, 1503.1010, 1503.9812,
	C	2.29662719	-0.43478224	0.27900488	1511.7091, 1512.5511, 1679.1572,
	H	2.67241247	0.51902015	-0.09838911	3029.8457, 3043.1925, 3045.6790,
	H	2.34265232	-0.38112112	1.37042153	3052.2609, 3054.6429, 3057.4794,
	C	3.17867293	-1.57260280	-0.21732198	3058.3509, 3067.6234, 3079.2127,
	H	3.15993848	-1.62822145	-1.30654573	3090.5825, 3099.0705, 3124.1143,
	H	2.83105856	-2.53180740	0.16903073	3126.3917, 3132.7298, 3132.9461,
	H	4.21472480	-1.44204878	0.09281420	3783.8687
	O	1.10194996	2.82231103	-0.23881629	
	H	1.55495256	2.88009635	0.61764085	
SP4_8	C	-3.66318717	-0.72532891	-0.26671054	639.7445i, 53.4279, 64.3782, 69.1810,
	H	-3.70685201	-0.47421579	-1.32746665	72.9702, 93.9268, 127.9353, 130.4730,
	H	-4.19880565	-1.66283264	-0.12262972	206.9791, 238.5169, 247.3229,
	H	-4.19618357	0.05370520	0.27994240	257.0971, 309.2581, 407.2112,
	C	-1.45166886	0.47719236	-0.00451033	503.4625, 646.0710, 730.1065,
	H	-1.41936304	0.69985890	-1.07663323	744.3509, 787.9233, 855.3374,
	H	-2.00727896	1.29085120	0.47000464	885.0185, 918.8022, 930.8385,
	C	-2.21857354	-0.82735370	0.20491622	987.8966, 1046.9109, 1059.1886,
	H	-2.19113985	-1.09037320	1.26564247	1075.3573, 1094.7260, 1116.3002,
	H	-1.71600041	-1.63598852	-0.32860726	1146.8167, 1185.8974, 1232.5163,
	C	-0.03662102	0.44566947	0.54500085	1256.2861, 1281.9579, 1294.9214,
	H	-0.04032608	0.30425378	1.62992648	1322.7406, 1330.9780, 1333.6315,
	H	0.42530900	1.48813404	0.40915350	1375.3284, 1388.2381, 1392.6087,
	C	0.90859021	-0.52930125	-0.12955900	1408.6897, 1413.1102, 1414.0891,
	H	0.86823090	-0.37569022	-1.21286674	1479.4740, 1485.6302, 1496.6880,
	H	0.56874087	-1.55436676	0.05193160	1497.4033, 1504.0620, 1504.2136,
	C	2.34798126	-0.38623417	0.34997272	1511.3553, 1512.1912, 1699.7002,
	H	2.67946877	0.63718998	0.16250269	
SP4_9	C	-3.66318717	-0.72532891	-0.26671054	639.7445i, 53.4279, 64.3782, 69.1810,
	H	-3.70685201	-0.47421579	-1.32746665	72.9702, 93.9268, 127.9353, 130.4730,
	H	-4.19880565	-1.66283264	-0.12262972	206.9791, 238.5169, 247.3229,
	H	-4.19618357	0.05370520	0.27994240	257.0971, 309.2581, 407.2112,
	C	-1.45166886	0.47719236	-0.00451033	503.4625, 646.0710, 730.1065,
	H	-1.41936304	0.69985890	-1.07663323	744.3509, 787.9233, 855.3374,
	H	-2.00727896	1.29085120	0.47000464	885.0185, 918.8022, 930.8385,
	C	-2.21857354	-0.82735370	0.20491622	987.8966, 1046.9109, 1059.1886,
	H	-2.19113985	-1.09037320	1.26564247	1075.3573, 1094.7260, 1116.3002,
	H	-1.71600041	-1.63598852	-0.32860726	1146.8167, 1185.8974, 1232.5163,
	C	-0.03662102	0.44566947	0.54500085	1256.2861, 1281.9579, 1294.9214,
	H	-0.04032608	0.30425378	1.62992648	1322.7406, 1330.9780, 1333.6315,
	H	0.42530900	1.48813404	0.40915350	1375.3284, 1388.2381, 1392.6087,
	C	0.90859021	-0.52930125	-0.12955900	1408.6897, 1413.1102, 1414.0891,
	H	0.86823090	-0.37569022	-1.21286674	1479.4740, 1485.6302, 1496.6880,
	H	0.56874087	-1.55436676	0.05193160	1497.4033, 1504.0620, 1504.2136,
	C	2.34798126	-0.38623417	0.34997272	1511.3553, 1512.1912, 1699.7002,
	H	2.67946877	0.63718998	0.16250269	

	H	2.37929342	-0.53026957	1.43309169	3027.8462, 3029.2854, 3052.1775,
	C	3.28799086	-1.37313236	-0.32888631	3053.8259, 3054.4070, 3057.3920,
	H	3.28642392	-1.22742690	-1.41004369	3058.0202, 3063.5622, 3075.2144,
	H	2.98152703	-2.40189666	-0.13325618	3093.9774, 3096.3246, 3123.7718,
	H	4.31256471	-1.25657007	0.02213738	3125.6773, 3133.4645, 3133.6014,
	O	0.85947817	2.79187377	-0.20110654	3784.3552
	H	0.05149524	2.91157851	-0.72531868	
SP4_10	C	-3.26963461	-0.76819325	-0.50286614	603.6182i, 52.0024, 60.4924, 73.9409,
	H	-3.01709818	-0.87027079	-1.55932285	84.3895, 102.7793, 121.2351,
	H	-3.84722006	-1.64430697	-0.21065881	202.3535, 209.4593, 243.6509,
	H	-3.91149996	0.10758467	-0.39931062	257.1230, 273.2774, 310.9230,
	C	-1.18311934	0.59684731	-0.06852144	419.3191, 525.1569, 651.5531,
	H	-0.86210054	0.47201845	-1.10721001	726.3591, 752.7405, 796.2837,
	H	-1.82156926	1.48406157	-0.04566773	853.4242, 888.2910, 896.6606,
	C	-2.01037586	-0.61992088	0.34067758	935.1849, 969.7615, 1051.0891,
	H	-2.27690229	-0.53289139	1.39736010	1062.2518, 1068.4628, 1074.2432,
	H	-1.40044828	-1.52153166	0.24959052	1127.0077, 1148.9252, 1168.9703,
	C	0.02473575	0.83219871	0.82395864	1228.7602, 1256.7855, 1281.3779,
	H	-0.29186804	1.13682285	1.82425304	1303.7290, 1325.1873, 1326.7190,
	H	0.58941176	1.74857522	0.42492915	1331.0974, 1372.2237, 1387.2685,
	C	1.03351988	-0.30269365	0.89762139	1402.1998, 1407.4412, 1412.8888,
	H	0.58835376	-1.14960209	1.43135819	1413.5958, 1482.5658, 1490.7983,
	H	1.88306466	0.02250564	1.50279439	1492.9937, 1500.4902, 1503.4217,
	C	1.54056311	-0.77218934	-0.46097997	1504.1292, 1509.7807, 1515.4509,
	H	0.71437187	-1.19491162	-1.03799482	1677.9520, 3031.0443, 3038.7941,
	H	1.90275612	0.09501673	-1.01934537	3048.9676, 3053.5160, 3057.3790,
	C	2.64805709	-1.80972917	-0.33160857	3058.2836, 3065.7988, 3072.6421,
H	2.29914811	-2.68284147	0.22216526	3080.7047, 3089.6357, 3094.9095,	
H	3.50308790	-1.39751282	0.20553432	3123.6928, 3124.8201, 3132.9838,	
H	2.99630297	-2.14896003	-1.30640955	3134.0313, 3784.0548	
O	1.21084834	2.80292120	-0.44938498		
H	0.56294666	2.71495575	-1.16667429		
SP4_11	C	-3.34215568	-0.00142239	-0.61149222	472.3042i, 37.2136, 67.3873, 82.6836,
	H	-3.09606570	-0.44536640	-1.57710323	101.5999, 108.9710, 123.4123,
	H	-4.21498565	-0.52012343	-0.21662856	189.4101, 225.6009, 254.3907,
	H	-3.61972239	1.03863965	-0.78750242	290.3176, 323.4926, 360.6389,
	C	-0.92396736	0.62389655	-0.20756072	431.6846, 509.9921, 630.6164,
	H	-0.62837718	0.15925969	-1.15190063	744.3780, 770.7150, 807.8724,
	H	-1.18777171	1.65702984	-0.44670268	848.0587, 880.9265, 889.7773,
	C	-2.15686917	-0.09235758	0.34065838	951.3216, 972.7755, 1033.6670,
	H	-2.42263791	0.33996851	1.30921756	1050.3550, 1059.0956, 1069.8016,
	H	-1.91717527	-1.14159206	0.52680430	1120.3774, 1162.2856, 1168.9245,
	C	0.24828339	0.62162896	0.75943774	1198.5424, 1252.1854, 1271.9957,
	H	0.01267604	1.21349807	1.64725581	1297.9344, 1312.2648, 1320.3219,
	H	1.10860301	1.17972400	0.24963101	1327.5086, 1363.7849, 1377.5245,
	C	0.77603206	-0.74743558	1.16985429	1386.4771, 1402.1920, 1412.3034,
	H	0.04613317	-1.21875860	1.83494399	1421.6233, 1479.6997, 1484.8559,
	H	1.68341453	-0.60706632	1.76232628	1495.3339, 1500.9711, 1503.0390,
	C	1.07964014	-1.68461343	0.00310878	1505.7015, 1511.0890, 1514.6941,
	H	1.44060428	-2.63246564	0.40626225	1736.8485, 3041.3827, 3046.5287,
	H	0.15613657	-1.91647570	-0.53369285	3052.7257, 3056.7268, 3059.0413,
	C	2.10992877	-1.11639096	-0.96668258	3062.1937, 3067.7539, 3077.8248,
H	3.02327761	-0.83620113	-0.43962435	3081.5717, 3090.8137, 3099.2659,	
H	1.74231559	-0.21976903	-1.46556668	3126.0610, 3128.8758, 3132.8200,	
H	2.37018812	-1.84503809	-1.73358399	3137.8130, 3787.0163	
O	2.11568727	2.15690367	-0.31520823		
H	1.83253573	2.91967390	0.21358794		
SP4_12	C	2.71331507	-1.26109944	-0.64133469	628.5997i, 49.7882, 62.8322, 73.9252,

	H	3.21522932	-0.59816728	-1.34846713	78.4698, 113.0941, 131.3603,
	H	3.37794274	-2.09958439	-0.43762377	146.5705, 195.9223, 247.3085,
	H	1.82413029	-1.65674637	-1.13331601	249.5590, 286.9055, 385.4012,
	C	1.53610037	0.75192774	0.39065611	404.7825, 484.6244, 648.9613,
	H	1.30031237	1.21247114	1.35456486	721.8087, 746.7168, 798.5993,
	H	2.14981168	1.46684773	-0.16423517	860.0890, 867.0155, 919.5350,
	C	2.35643798	-0.51678373	0.63965411	932.9264, 972.3056, 1033.4353,
	H	1.80560416	-1.18046099	1.30920095	1047.2286, 1075.2463, 1094.8816,
	H	3.27035243	-0.23950450	1.16768152	1122.9684, 1148.0402, 1177.0667,
	C	0.24136309	0.51120722	-0.36870767	1229.6240, 1251.2526, 1282.2109,
	H	0.42946998	0.22717999	-1.40731397	1293.2057, 1308.4265, 1332.8611,
	H	-0.30768100	1.51490220	-0.46230471	1362.1678, 1372.3152, 1383.6697,
	C	-0.73058828	-0.44568402	0.29248193	1391.2960, 1408.6604, 1413.8077,
	H	-0.87425229	-0.14771772	1.33618179	1416.6792, 1478.2639, 1488.2707,
	H	-0.29442842	-1.45087440	0.31496683	1496.9914, 1497.5872, 1503.8092,
	C	-2.08058828	-0.50044368	-0.41211752	1505.3447, 1510.6778, 1512.4321,
	H	-2.50900314	0.50389467	-0.42697183	1691.2648, 3024.1044, 3037.8750,
	H	-1.92727497	-0.78867378	-1.45539800	3050.4818, 3055.2636, 3056.2680,
	C	-3.04597938	-1.47095106	0.25460537	3058.3574, 3061.2740, 3071.3809,
	H	-3.22829011	-1.18389595	1.29116072	3083.1604, 3093.4212, 3096.0378,
	H	-2.64057307	-2.48397837	0.25825796	3123.5254, 3124.1936, 3133.5334,
	H	-4.00645955	-1.49660703	-0.25859069	3133.6134, 3783.8337
	O	-0.92046613	2.85221177	-0.15348756	
	H	-0.16152486	3.17418278	0.35868125	
	C	-3.35309843	-0.01883651	-0.61874760	
	H	-3.09623527	-0.50495432	-1.56104096	535.7680i, 47.6466, 68.5845, 105.2395,
	H	-4.22419505	-0.52648939	-0.20609411	119.3080, 131.7162, 158.1589,
	H	-3.63807660	1.00940261	-0.84465282	191.4686, 243.2475, 279.0250,
	C	-0.94526649	0.65289230	-0.22510552	291.8252, 324.6104, 354.8589,
	H	-0.64688796	0.15961811	-1.15438715	424.0680, 529.1581, 659.2432,
	H	-1.21517336	1.67586086	-0.49621494	742.0180, 758.2091, 795.5170,
	C	-2.17419652	-0.05426869	0.34493952	837.4266, 879.5713, 892.4579,
	H	-2.45171367	0.41822609	1.29090166	947.3212, 955.8243, 1037.6794,
	H	-1.92514285	-1.09166063	0.58011143	1053.9812, 1063.1735, 1071.1390,
	C	0.22184868	0.69165752	0.74586714	1125.9057, 1154.6544, 1172.7926,
	H	-0.02823168	1.29552513	1.62102500	1214.0426, 1250.4107, 1263.0947,
	H	1.05499184	1.31020756	0.25274163	1285.8167, 1308.0388, 1323.5197,
	C	0.77203117	-0.65807090	1.18863353	1327.7651, 1367.3314, 1380.6942,
	H	0.06414480	-1.10719252	1.89134629	1389.2149, 1403.0772, 1410.3730,
	H	1.69302678	-0.49253558	1.75417823	1412.6162, 1480.8068, 1485.3531,
	C	1.04389939	-1.65165524	0.06093485	1496.7057, 1502.7373, 1505.4127,
	H	1.40131879	-2.58461359	0.49977569	1506.2997, 1514.2793, 1521.0678,
	H	0.10903070	-1.89499850	-0.44938631	1633.0165, 3041.0198, 3043.8008,
	C	2.06097030	-1.15196898	-0.95857529	3046.9754, 3055.0359, 3058.2692,
	H	2.99992553	-0.88649211	-0.46508198	3060.8968, 3072.9139, 3076.0532,
	H	1.69248239	-0.27471576	-1.49217861	3082.3077, 3092.2200, 3099.6811,
	H	2.28748614	-1.91696046	-1.70007688	3116.1929, 3125.4925, 3132.6330,
	O	2.17536666	2.14501779	-0.28584793	3133.3783, 3784.5051
	H	2.76318749	1.39313325	-0.46186246	
	C	-2.89065365	-0.84150850	0.47838932	
	H	-3.53356414	0.02822773	0.62512957	599.9195i, 32.3045, 60.1931, 63.5249,
	H	-3.53046346	-1.71270216	0.34424638	80.2171, 104.6899, 117.6116,
	H	-2.31982607	-0.98901300	1.39556820	185.3693, 213.8074, 251.8222,
	C	-1.14568679	0.64395681	-0.63978382	276.1897, 288.2641, 361.8713,
	H	-0.52516465	0.72199736	-1.53619514	425.0327, 531.6681, 652.6837,
	H	-1.82048482	1.50395355	-0.64872326	728.5228, 750.3426, 805.8061,
	C	-1.97452814	-0.64015848	-0.72295327	844.8655, 885.3857, 894.7228,
	H	-1.30644904	-1.49900373	-0.82297231	938.5042, 961.5102, 1030.1707,
SP4_13					
SP4_14					

	H	-2.57160504	-0.60928885	-1.63589555	1061.0573, 1065.8057, 1075.9561,
	C	-0.26432529	0.72482391	0.59878271	1127.0194, 1150.5509, 1166.0062,
	H	-0.86365169	0.88416858	1.49707040	1221.2024, 1250.5241, 1280.4288,
	H	0.36192922	1.68427877	0.52371258	1298.3492, 1317.9468, 1327.4759,
	C	0.71315236	-0.42242990	0.79239969	1357.2607, 1369.5283, 1382.8775,
	H	0.15547043	-1.34164274	1.00686884	1404.7321, 1408.9305, 1412.6150,
	H	1.31898881	-0.22283800	1.67937239	1417.0350, 1476.4868, 1490.6157,
	C	1.63624422	-0.65948093	-0.39753620	1498.0805, 1499.5404, 1504.0394,
	H	1.04777129	-0.95476239	-1.26940837	1505.4930, 1511.4397, 1512.1782,
	H	2.12640443	0.28340181	-0.65352841	1665.5012, 3025.5453, 3045.8294,
	C	2.68080812	-1.72936899	-0.10754071	3052.5513, 3055.4672, 3057.3951,
	H	2.20490766	-2.67812958	0.14574088	3059.8018, 3071.9347, 3079.0954,
	H	3.30801289	-1.43853567	0.73603429	3089.5098, 3091.8669, 3097.9496,
	H	3.33037151	-1.89939057	-0.96528325	3123.8500, 3125.5522, 3132.6938,
	O	1.16492541	2.86199561	0.05032834	3134.9639, 3782.8651
	H	0.76788427	2.88831059	-0.83491021	
	C	-3.03872794	0.31122928	-0.35377879	
	H	-2.73388636	0.65901181	-1.34218966	551.8028i, 43.3580, 60.7012, 70.5718,
	H	-4.12717683	0.27359148	-0.32844411	85.0796, 104.0364, 129.0533,
	H	-2.71156331	1.06123414	0.36557415	138.7587, 232.2449, 238.7105,
	C	-0.91632343	-1.08363719	-0.19447511	262.3844, 290.7908, 308.9285,
	H	-0.54726984	-2.09927503	-0.01238295	418.8648, 526.3546, 655.8395,
	H	-0.64554065	-0.83598176	-1.22418485	735.8737, 764.6704, 781.3196,
	C	-2.43548250	-1.05662414	-0.05384208	845.1060, 866.6033, 905.4849,
	H	-2.70582293	-1.36364721	0.96010112	941.5201, 965.5889, 1038.1689,
	H	-2.86551185	-1.80069335	-0.72679230	1059.3309, 1071.2349, 1091.0892,
	C	-0.20102080	-0.13958060	0.75764009	1124.2301, 1164.3615, 1169.9533,
	H	-0.64783471	-0.18279714	1.75459915	1227.2917, 1264.9694, 1273.5267,
	H	-0.41686810	0.92891498	0.39927222	1292.2864, 1310.6995, 1325.6400,
	C	1.30653979	-0.31436131	0.83070002	1337.2079, 1372.8125, 1376.7973,
	H	1.52825111	-1.29423544	1.26829040	1399.6503, 1407.3213, 1414.6677,
	H	1.72413931	0.42463637	1.52155737	1421.4902, 1479.6557, 1483.9555,
	C	2.01477641	-0.19851017	-0.51542633	1492.0062, 1498.4986, 1504.0683,
	H	1.69244214	-1.01213041	-1.16772621	1504.2984, 1512.0383, 1514.2636,
	H	1.70319975	0.72826923	-1.00521378	1677.3582, 3024.2925, 3028.1432,
	C	3.53055850	-0.23372665	-0.37149575	3048.1986, 3052.3887, 3056.3358,
	H	3.85313558	-1.16012253	0.10620116	3057.5036, 3062.3361, 3064.5986,
	H	3.88294170	0.59434954	0.24544822	3077.8382, 3089.5550, 3093.9962,
	H	4.02721432	-0.16545765	-1.33849086	3122.2858, 3129.2246, 3134.1851,
	O	-0.37984372	2.36878104	-0.05488279	3139.4394, 3780.5233
	H	0.46698016	2.58534939	0.36751093	
	C	-2.75231752	0.54261732	-0.40948728	
	H	-2.33929775	0.93828031	-1.33903556	572.6667i, 42.8705, 76.8320, 89.9839,
	H	-3.83755867	0.62354678	-0.45972955	115.1326, 131.1320, 154.7235,
	H	-2.40307058	1.18678801	0.39637232	195.6586, 234.0533, 255.5672,
	C	-0.80784549	-1.09410933	-0.24921256	298.8944, 315.9431, 354.1180,
	H	-0.56862893	-2.15652299	-0.12597909	438.8311, 516.9881, 663.0867,
	H	-0.44022598	-0.81185898	-1.24025883	727.3448, 776.0397, 796.2234,
	C	-2.32098172	-0.90433666	-0.19936060	839.7843, 852.9590, 907.4161,
	H	-2.69197358	-1.26150224	0.76505335	949.2671, 955.8954, 1017.2289,
	H	-2.78037660	-1.53768046	-0.96052998	1046.4464, 1068.3064, 1093.9416,
	C	-0.05799770	-0.31358815	0.81706426	1113.7801, 1142.8881, 1156.9279,
	H	-0.58536185	-0.36161611	1.77322364	1181.0994, 1247.5999, 1264.1881,
	H	-0.12537048	0.80660674	0.55567855	1296.9290, 1303.8330, 1321.4974,
	C	1.39993143	-0.70933554	1.00423711	1353.1416, 1376.7402, 1378.8969,
	H	1.42110150	-1.68775875	1.49421256	1388.4695, 1407.3814, 1411.0603,
	H	1.87543955	-0.01024130	1.69818665	1421.0556, 1474.4085, 1482.8901,
	C	2.22361197	-0.78981416	-0.27997563	1491.1507, 1498.5866, 1503.1183,
SP4_15					
SP4_16					

	H	3.22635979	-1.13822635	-0.02707365	1506.5450, 1510.1304, 1517.3893,
	H	1.79638072	-1.54726429	-0.94022283	1639.1886, 3025.4906, 3035.4909,
	C	2.32381222	0.53508986	-1.02628634	3043.6173, 3047.3545, 3060.6124,
	H	2.76430831	1.30491094	-0.38659539	3061.6805, 3065.0469, 3074.1970,
	H	1.34513162	0.88584512	-1.35621248	3076.8719, 3089.2168, 3094.6253,
	H	2.95809384	0.44506622	-1.90721506	3116.5095, 3128.0058, 3134.8961,
	O	-0.07000455	2.29668578	0.46647913	3142.4667, 3784.2937
	H	0.89580636	2.34900103	0.38641849	
SP4_17	C	-3.06910251	0.09483396	0.37319232	487.4575i, 46.1565, 75.3450, 92.8705,
	H	-3.33076596	1.14537748	0.23357356	95.1860, 121.0296, 130.8562,
	H	-3.99061154	-0.48551640	0.35082112	200.1792, 210.4996, 260.8025,
	H	-2.63850868	-0.00950834	1.36957868	322.5095, 336.4629, 386.2997,
	C	-0.84350738	0.50260535	-0.80663286	442.1371, 516.2322, 632.0786,
	H	-0.20418977	0.12468416	-1.60715046	744.6781, 773.7550, 815.8519,
	H	-1.13496801	1.51484891	-1.09754649	833.6288, 880.1982, 885.4906,
	C	-2.09829815	-0.36917271	-0.70637363	950.9716, 977.8037, 1010.2135,
	H	-1.81005673	-1.40586534	-0.51759781	1041.7424, 1057.9206, 1075.3250,
	H	-2.60096198	-0.36321585	-1.67504354	1113.3217, 1159.3803, 1165.6326,
	C	-0.04554759	0.57420573	0.48662445	1187.9789, 1243.3936, 1264.5412,
	H	-0.58489985	1.13752511	1.25056377	1292.9558, 1304.2095, 1320.4026,
	H	0.88761516	1.20302728	0.26801256	1349.3263, 1367.8575, 1378.9481,
	C	0.42332542	-0.75969296	1.05162947	1381.8464, 1401.8201, 1414.6466,
	H	-0.44924657	-1.30520581	1.42617595	1420.5789, 1475.5131, 1485.4689,
	H	1.05938905	-0.56767408	1.91908256	1497.6645, 1498.9219, 1503.5738,
	C	1.18202291	-1.63890530	0.05926247	1506.9008, 1510.6506, 1513.9947,
	H	1.45947017	-2.56673345	0.56271150	1736.9511, 3035.7913, 3054.0286,
	H	0.52017153	-1.92587355	-0.76147024	3056.2175, 3058.2508, 3060.9589,
C	2.43163521	-0.96774605	-0.50001459	3062.2461, 3076.6449, 3079.2572,	
H	3.08171838	-0.62638121	0.30712513	3091.5042, 3092.0218, 3101.8810,	
H	2.18457400	-0.09357544	-1.10214262	3124.5179, 3128.9366, 3133.7515,	
H	2.99933133	-1.65636275	-1.12477441	3138.3831, 3784.9686	
O	1.91007329	2.28120290	0.00982907		
H	1.38818567	3.01405793	0.37332244		
SP4_18	C	-3.39273364	-0.53944246	-0.41673989	476.4659i, 43.0619, 55.1384, 60.4685,
	H	-3.18631181	-0.77940722	-1.46069993	77.7604, 80.9496, 115.2837, 201.9667,
	H	-4.03239128	-1.32322425	-0.01253994	208.2246, 247.1358, 258.2840,
	H	-3.95334315	0.39596090	-0.39759201	303.6469, 309.6537, 425.0863,
	C	-1.18397965	0.67383412	-0.19813670	514.5583, 634.6661, 732.4347,
	H	-0.90480556	0.40751663	-1.22042060	749.9635, 814.3276, 854.9004,
	H	-1.74171778	1.61050841	-0.26791644	887.3404, 892.4839, 955.9772,
	C	-2.09651607	-0.41035277	0.37253281	971.8488, 1038.3227, 1052.9458,
	H	-2.31806592	-0.18153340	1.41859253	1065.6856, 1069.8689, 1118.0970,
	H	-1.57066021	-1.36785253	0.37093249	1165.6184, 1170.7652, 1211.7915,
	C	0.06670594	0.90272631	0.63600435	1254.1674, 1275.3441, 1310.2677,
	H	-0.19008565	1.35959592	1.59475674	1317.5454, 1326.4147, 1329.1675,
	H	0.69075913	1.68276921	0.07732152	1372.3623, 1380.5809, 1393.1908,
	C	0.96873361	-0.30405134	0.84077643	1406.2273, 1411.9655, 1412.8060,
	H	0.46102975	-1.03661127	1.47749606	1481.1820, 1490.5018, 1491.8663,
	H	1.85789906	0.01206583	1.39228489	1500.2972, 1503.2303, 1503.9377,
	C	1.40340871	-0.97369798	-0.45759369	1509.2769, 1514.5944, 1704.1557,
	H	0.53016122	-1.38148886	-0.97229230	3031.8661, 3046.5567, 3051.0422,
	H	1.82998241	-0.21480829	-1.11834321	3056.0982, 3057.4279, 3059.9276,
	C	2.41462348	-2.08695249	-0.21774503	3066.9810, 3071.9924, 3079.6180,
H	1.99970857	-2.85415128	0.43810848	3090.4634, 3100.7802, 3122.7832,	
H	3.31461751	-1.69605880	0.25871705	3125.7908, 3132.4906, 3132.8404,	
H	2.71068262	-2.56767825	-1.14933006	3785.1203	
O	1.69911221	2.65070917	-0.51131819		
H	1.82818912	3.15634360	0.30688061		

SP4_19	C	-3.09455790	0.13907967	0.37762819	541.4549i, 56.4732, 82.6041, 95.1819, 117.6571, 145.7677, 168.4803, 199.1524, 236.2895, 291.2080, 322.2329, 330.5853, 382.4670, 442.6549, 530.9427, 660.0489, 740.9187, 751.2393, 801.4326, 831.1154, 881.8321, 886.9136, 946.7923, 955.9731, 1011.5075, 1053.3089, 1063.7696, 1075.1789, 1118.9256, 1155.6817, 1171.0564, 1199.5511, 1239.7733, 1251.9160, 1288.4500, 1301.0119, 1310.5760, 1353.9107, 1365.5438, 1382.0341, 1386.7599, 1403.5224, 1410.4747, 1416.5861, 1476.3026, 1485.6457, 1497.8480, 1501.9192, 1506.0921, 1509.7328, 1510.9722, 1521.1108, 1639.6609, 3035.3927, 3043.6865, 3056.2419, 3057.5761, 3060.2806, 3062.7875, 3073.7979, 3085.6166, 3091.1903, 3094.0170, 3104.1336, 3116.9839, 3126.2480, 3133.6257, 3134.1518, 3784.5097
	H	-3.35952380	1.18017389	0.18523716	
	H	-4.01380325	-0.44521539	0.38662285	
	H	-2.66172923	0.08758953	1.37709793	
	C	-0.87511154	0.49716119	-0.83121468	
	H	-0.24152542	0.08414850	-1.61937704	
	H	-1.17394517	1.49291976	-1.16573475	
	C	-2.12467707	-0.37606872	-0.67942045	
	H	-1.83097026	-1.40015906	-0.43686891	
	H	-2.63071475	-0.42371526	-1.64517972	
	C	-0.07124249	0.63550967	0.45169261	
	H	-0.61578639	1.21824618	1.19644289	
	H	0.81799764	1.32465145	0.21505285	
	C	0.42422384	-0.66458259	1.06915600	
	H	-0.43321286	-1.18816825	1.50426477	
	H	1.08727037	-0.42697416	1.90544581	
	C	1.14296968	-1.61140015	0.10927700	
	H	1.41833398	-2.51483157	0.65591095	
	H	0.45668915	-1.93004763	-0.67825539	
	C	2.38993366	-1.00537706	-0.52407830	
H	3.08186231	-0.65650039	0.24743376		
H	2.14006933	-0.16182445	-1.16887407		
H	2.92093729	-1.73765875	-1.13085626		
O	1.95528547	2.27617823	0.02617699		
H	2.64653828	1.60200775	0.12397900		
SP4_20	C	3.69988064	-0.37390942	0.01597703	612.6892i, 36.0495, 63.5421, 66.3558, 78.4277, 90.6328, 110.8340, 130.3690, 230.2904, 238.6452, 256.3905, 287.4530, 312.1231, 410.8151, 527.3487, 651.9939, 739.2656, 758.4057, 794.2432, 844.5143, 882.4180, 904.7304, 938.3807, 966.5340, 1048.6390, 1055.0450, 1072.0118, 1089.4121, 1120.6675, 1147.5206, 1172.6242, 1229.3037, 1254.9554, 1281.3078, 1304.7489, 1316.5055, 1328.0895, 1346.3717, 1375.3034, 1390.0333, 1391.3333, 1407.0186, 1412.7695, 1415.9112, 1481.7828, 1486.5630, 1494.5901, 1496.9771, 1503.8149, 1504.2094, 1511.6724, 1512.9509, 1681.2081, 3027.7726, 3031.1728, 3052.1305, 3054.7588, 3058.0117, 3059.4388, 3063.2522, 3070.3558, 3085.4000, 3095.2451, 3098.2462, 3125.1326, 3125.4789, 3133.9640, 3135.9947, 3781.8496
	H	3.88149907	0.13681855	0.96272839	
	H	4.32353026	-1.26670831	-0.00742174	
	H	4.03027688	0.28785762	-0.78571633	
	C	1.33628994	0.52526821	-0.09538259	
	H	1.45222979	1.00868094	0.88074867	
	H	1.69144974	1.23741826	-0.84547195	
	C	2.22407050	-0.71721995	-0.13771304	
	H	2.05989353	-1.24018125	-1.08362654	
	H	1.92362084	-1.40618004	0.65387249	
	C	-0.13231547	0.22507066	-0.33703697	
	H	-0.28399811	-0.16614370	-1.34600857	
	H	-0.71022511	1.21718340	-0.34091817	
	C	-0.79186112	-0.65619105	0.70947480	
	H	-0.47683026	-0.32039721	1.70140810	
	H	-0.42590681	-1.68214655	0.59488950	
	C	-2.31728124	-0.65705071	0.63358482	
	H	-2.70877231	-1.28742351	1.43386209	
	H	-2.67705085	0.35645147	0.82292698	
	C	-2.85304729	-1.14681388	-0.70703152	
H	-2.44414317	-2.12841804	-0.95538637		
H	-2.59282831	-0.46141567	-1.51342645		
H	-3.93881291	-1.23172055	-0.68815679		
O	-1.21760845	2.60182076	-0.03061673		
H	-0.35748046	2.93683541	0.26939540		
SP4_21	C	3.16133803	-0.25190430	-0.08945446	650.6831i, 38.5189, 55.6289, 75.0974, 90.4505, 105.7036, 136.2900, 148.9621, 228.2324, 244.3460, 256.3965, 287.6450, 296.8280, 401.4506, 526.4576, 654.4788, 727.4903, 743.2064, 783.2886, 849.4760, 883.7393, 903.4351,
	H	3.23751403	0.25058900	0.87586565	
	H	4.14748160	-0.63144780	-0.35479391	
	H	2.88553316	0.50441403	-0.82330053	
	C	0.76848936	-0.94093220	0.47290589	
	H	0.11376294	-1.81501205	0.53102041	
	H	0.85978125	-0.55101048	1.49158043	
	C	2.13998273	-1.38247480	-0.03215708	

	H	2.02641721	-1.82584427	-1.02515749	935.2168, 968.7731, 1044.5244,
	H	2.51231539	-2.17653454	0.61769659	1056.9813, 1071.4220, 1088.2244,
	C	0.10505749	0.11504176	-0.39268514	1115.8583, 1141.5123, 1183.5812,
	H	0.14856984	-0.15541629	-1.45262636	1218.8103, 1254.8002, 1285.9688,
	H	0.75072533	1.06153968	-0.31818407	1296.7811, 1312.4667, 1327.2998,
	C	-1.30982606	0.49201519	0.01421745	1348.2610, 1371.6441, 1380.3460,
	H	-1.62251898	1.37848332	-0.54619626	1391.5000, 1403.9887, 1412.4554,
	H	-1.31911264	0.76923671	1.07359402	1421.9239, 1476.3951, 1485.9963,
	C	-2.33976789	-0.61078753	-0.22403277	1491.2092, 1496.4387, 1502.3040,
	H	-2.29188719	-0.92176918	-1.27078385	1503.3068, 1511.3719, 1511.7435,
	H	-2.08642289	-1.48848914	0.37254877	1716.9763, 3029.3053, 3036.2299,
	C	-3.75325442	-0.15640614	0.11651643	3047.1877, 3052.0258, 3054.4327,
	H	-4.04359057	0.69999212	-0.49356198	3058.1708, 3063.7237, 3066.1261,
	H	-3.82145016	0.14428291	1.16293986	3079.2898, 3088.4685, 3097.8530,
	H	-4.48032231	-0.94986243	-0.05173410	3125.8242, 3131.1995, 3133.9593,
	O	1.24760853	2.41650654	0.09262006	3138.7038, 3782.5844
	H	0.37022033	2.78748428	0.27827038	
	C	2.88352236	-0.78966332	-0.71278430	681.8959i, 44.9725, 57.1094, 87.8950,
	H	3.03344748	-0.16161807	-1.59289714	105.1438, 125.7670, 153.6447,
	H	3.79876228	-1.35560339	-0.54401478	182.6112, 224.6620, 271.5146,
	H	2.09291154	-1.50361036	-0.94813070	281.1650, 318.9772, 350.1650,
	C	1.33638773	0.99245053	0.25894145	428.9636, 510.1565, 652.0033,
	H	1.09309554	1.52022902	1.18380591	722.5674, 753.4250, 792.5839,
	H	1.62705547	1.75591358	-0.46626609	851.2447, 868.2152, 902.2928,
	C	2.52458014	0.05746616	0.50226745	927.8488, 960.7797, 1018.9762,
	H	2.31685668	-0.59325432	1.35397569	1048.2398, 1073.2391, 1095.6833,
	H	3.38388135	0.66557324	0.78987225	1112.7397, 1144.8005, 1170.1151,
	C	0.08225253	0.29886783	-0.24925803	1218.5122, 1247.2797, 1289.0261,
	H	0.21701780	-0.09638982	-1.26026426	1290.6374, 1306.6641, 1335.0425,
	H	-0.68084862	1.14891233	-0.38190175	1357.7690, 1372.0594, 1381.7172,
	C	-0.49215795	-0.75633641	0.67740180	1386.8054, 1405.1924, 1412.9615,
	H	-0.80295303	-0.27884996	1.61267405	1416.3411, 1479.3014, 1487.0491,
	H	0.30363136	-1.45824428	0.94333894	1495.3336, 1497.9613, 1504.5422,
	C	-1.65476563	-1.54941223	0.08490932	1506.9457, 1511.6385, 1521.4479,
	H	-1.30804121	-2.06726255	-0.81323404	1655.5476, 3033.0532, 3043.2185,
	H	-1.94958764	-2.32533531	0.79337610	3050.9783, 3053.8292, 3055.7788,
	C	-2.87080904	-0.69871463	-0.26316942	3061.1543, 3063.3075, 3076.3958,
	H	-2.64839898	0.00700456	-1.06406970	3088.8064, 3090.5497, 3100.9885,
	H	-3.20983077	-0.13690180	0.61162508	3116.9156, 3122.1019, 3132.6808,
	H	-3.70339261	-1.31767027	-0.59497290	3134.3335, 3784.2264
	O	-1.51361040	2.37222583	-0.18807579	
	H	-2.30878432	1.89135312	0.09184015	
SP4_22					

Table S2. Computed energies of all the conformers of the stationary points involved in reactions R1-R4 at the M06-2X/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ

levels of theory with their associated T1 diagnostic values provided for the conformers whose energy is below 1 kcal mol⁻¹ of the corresponding global minimum

Conformer species	M06-2X/aug-cc-pVTZ (a.u.)	CCSD(T)/aug-cc-pVTZ (a.u.)	T1 diagnostic
OH	-75.7338102	-75.64558432	0.01003122
n-heptane_1	-276.3434533	-275.8931079	0.00856549
n-heptane_2	-276.3426196	-275.8922611	0.00859211
n-heptane_3	-276.3426146	-275.8922912	0.00859697
n-heptane_4	-276.3425076	-275.8919244	0.00863591
n-heptane_5	-276.3424915	-275.8919623	0.00863738
n-heptane_6	-276.3423942	-275.8915877	0.00867225
n-heptane_7	-276.3422352	-275.8911467	0.00870521
n-heptane_8	-276.3418984	-275.8912161	0.00866703
n-heptane_9	-276.3418970	-275.8914695	0.00862092
n-heptane_10	-276.3418223		
n-heptane_11	-276.3417331		
n-heptane_12	-276.3415217		
n-heptane_13	-276.3414424		
n-heptane_14	-276.3398265		
n-heptane_15	-276.3395971		
n-heptane_16	-276.3395555		
n-heptane_17	-276.3395412		
n-heptane_18	-276.3389862		
n-heptane_19	-276.3389114		
n-heptane_20	-276.3388698		
n-heptane_21	-276.3387555		
n-heptane_22	-276.3342010		
SP1_1	-352.0732280	-351.5339891	0.014884
SP1_2	-352.0730307	-351.5339220	0.014844
SP1_3	-352.0729165	-351.5330115	0.015212
SP1_4	-352.0725040	-351.5329163	0.015022
SP1_5	-352.0724867	-351.5330585	0.015134
SP1_6	-352.0723895	-351.5331335	0.014900
SP1_7	-352.0723875	-351.5331449	0.014897
SP1_8	-352.0723787	-351.5331313	0.014906
SP1_9	-352.0723707	-351.5331795	0.014902
SP1_10	-352.0723677	-351.5332564	0.014907
SP1_11	-352.0723203	-351.5333274	0.014880
SP1_12	-352.0722969	-351.5333003	0.014892
SP1_13	-352.0722379	-351.5331209	0.014874
SP1_14	-352.0722268	-351.5331979	0.014866
SP1_15	-352.0722130	-351.5331373	0.014864
SP1_16	-352.0721930	-351.5330630	0.014861
SP1_17	-352.0720907	-351.5327737	0.014883
SP1_18	-352.0720872	-351.5327909	0.014895
SP1_19	-352.0719916	-351.5320522	0.015205
SP1_20	-352.0719908	-351.5320490	0.015179
SP1_21	-352.0718994	-351.5322067	0.015086
SP1_22	-352.0718005	-351.5315036	0.015215
SP1_23	-352.0717658	-351.5320972	0.015073
SP1_24	-352.0716881	-351.5317988	0.015053
SP1_25	-352.0716624	-351.5320407	0.015024
SP1_26	-352.0715386		
SP1_27	-352.0715371		
SP1_28	-352.0715241		

SP1_29	-352.0715153		
SP1_30	-352.0714966		
SP1_31	-352.0714911		
SP1_32	-352.0714763		
SP1_33	-352.0713661		
SP1_34	-352.0713633		
SP1_35	-352.0713595		
SP1_36	-352.0713571		
SP1_37	-352.0712773		
SP1_38	-352.0708026		
SP1_39	-352.0706655		
SP1_40	-352.0703639		
SP1_41	-352.0703242		
SP1_42	-352.0703059		
SP2_1	-352.0756664	-351.5370173	0.014911
SP2_2	-352.0756601	-351.5361257	0.015322
SP2_3	-352.0756597	-351.5361150	0.015321
SP2_4	-352.0756062	-351.5370213	0.014855
SP2_5	-352.0755877	-351.5367620	0.014954
SP2_6	-352.0749655	-351.5353118	0.015253
SP2_7	-352.0748378	-351.5355807	0.015166
SP2_8	-352.0748307	-351.5361661	0.014940
SP2_9	-352.0748161	-351.5362111	0.014935
SP2_10	-352.0748141	-351.5361648	0.014927
SP2_11	-352.0748141	-351.5361294	0.014992
SP2_12	-352.0747996	-351.5362316	0.014934
SP2_13	-352.0747736	-351.5359636	0.014971
SP2_14	-352.0747736	-351.5359632	0.014971
SP2_15	-352.0747670	-351.5359854	0.014966
SP2_16	-352.0747633	-351.5359370	0.014967
SP2_17	-352.0747178	-351.5359503	0.014981
SP2_18	-352.0747019	-351.5358416	0.014959
SP2_19	-352.0746473	-351.5355940	0.014990
SP2_20	-352.0746362	-351.5360589	0.014898
SP2_21	-352.0743720	-351.5355867	0.014970
SP2_22	-352.0742784	-351.5358223	0.014885
SP2_23	-352.0741451	-351.5347812	0.015166
SP2_24	-352.0740814	-351.5349327	0.014983
SP2_25	-352.0737586		
SP2_26	-352.0737030		
SP2_27	-352.0736788		
SP2_28	-352.0736444		
SP2_29	-352.0735953		
SP2_30	-352.0735760		
SP3_1	-352.0763550	-351.5378167	0.014995
SP3_2	-352.0758637	-351.5364675	0.015420
SP3_3	-352.0757075	-351.5367384	0.015211
SP3_4	-352.0756914	-351.5370370	0.015127
SP3_5	-352.0756004	-351.5366493	0.015134
SP3_6	-352.0755516	-351.5369720	0.015020
SP3_7	-352.0755082	-351.5357771	0.015514
SP3_8	-352.0754908	-351.5369593	0.015011
SP3_9	-352.0754114	-351.5368837	0.014995
SP3_10	-352.0753963	-351.5357998	0.015410
SP3_11	-352.0753873	-351.5368862	0.014995
SP3_12	-352.0753661	-351.5361827	0.015262

SP3_13	-352.0753289	-351.5362656	0.015160
SP3_14	-352.0751149	-351.5365935	0.015089
SP3_15	-352.0750939	-351.5364041	0.015080
SP3_16	-352.0750271	-351.5365339	0.015027
SP3_17	-352.0749427	-351.5359718	0.015117
SP3_18	-352.0749011	-351.5350043	0.015427
SP3_19	-352.0748824	-351.5360720	0.015055
SP3_20	-352.0748372	-351.5355104	0.015230
SP3_21	-352.0747307		
SP3_22	-352.0746027		
SP3_23	-352.0745289		
SP3_24	-352.0744558		
SP3_25	-352.0743532		
SP3_26	-352.0742770		
SP3_27	-352.0742379		
SP3_28	-352.0741487		
SP3_29	-352.0741193		
SP3_30	-352.0740857		
SP3_31	-352.0740635		
SP4_1	-352.0763276	-351.5378410	0.01499552
SP4_2	-352.0760624	-351.5371616	0.01507263
SP4_3	-352.0759582	-351.5366945	0.01530522
SP4_4	-352.0756856	-351.5366599	0.0152121
SP4_5	-352.0753854	-351.5369317	0.01499584
SP4_6	-352.0753185	-351.5363511	0.01516265
SP4_7	-352.0753101	-351.5360418	0.01526247
SP4_8	-352.0750852	-351.5366402	0.01507784
SP4_9	-352.0750801	-351.5364536	0.01508074
SP4_10	-352.0750323	-351.5361423	0.01512009
SP4_11	-352.0749985	-351.5360145	0.01515575
SP4_12	-352.0748772	-351.5360859	0.01505795
SP4_13	-352.0748678	-351.5355057	0.01526785
SP4_14	-352.0748575	-351.5357304	0.0151051
SP4_15	-352.0748284	-351.5357934	0.01518201
SP4_16	-352.0747824	-351.5350702	0.01539813
SP4_17	-352.0747763	-351.5355048	0.01516426
SP4_18	-352.0747655	-351.5362379	0.01505391
SP4_19	-352.0745459		
SP4_20	-352.0744227		
SP4_21	-352.0742420		
SP4_22	-352.0740296		

Table S3. Site-specific rate constants obtained with the SS-HO-LL approach

T (K)	k (cm ³ molecule ⁻¹ s ⁻¹)			
	R1	R2	R3	R4
200	1.30E-14	2.62E-13	5.87E-13	4.28E-13
298	5.63E-14	4.71E-13	1.04E-12	6.70E-13
400	1.58E-13	7.65E-13	1.70E-12	9.96E-13
500	3.29E-13	1.15E-12	2.53E-12	1.41E-12
600	5.83E-13	1.63E-12	3.58E-12	1.93E-12
700	9.32E-13	2.25E-12	4.86E-12	2.57E-12
800	1.39E-12	3.00E-12	6.40E-12	3.35E-12
900	1.97E-12	3.91E-12	8.20E-12	4.28E-12
1000	2.38E-12	4.99E-12	1.03E-11	5.38E-12
1100	3.16E-12	6.25E-12	1.27E-11	6.67E-12
1200	4.09E-12	7.72E-12	1.54E-11	8.14E-12
1300	5.18E-12	9.39E-12	1.85E-11	9.82E-12
1400	6.45E-12	1.13E-11	2.19E-11	1.17E-11
1500	7.91E-12	1.34E-11	2.56E-11	1.38E-11
1600	9.56E-12	1.58E-11	2.98E-11	1.62E-11
1800	1.35E-11	2.13E-11	3.93E-11	2.16E-11
2000	1.83E-11	2.80E-11	5.04E-11	2.81E-11
2200	2.41E-11	3.58E-11	6.33E-11	3.57E-11
2500	3.47E-11	4.99E-11	8.62E-11	4.94E-11
2800	4.79E-11	6.70E-11	1.13E-10	6.59E-11
3000	5.82E-11	8.01E-11	1.34E-10	7.85E-11

Table S4. Site-specific rate constants obtained with the SS-HO-HL approach

T (K)	k (cm ³ molecule ⁻¹ s ⁻¹)			
	R1	R2	R3	R4
200	5.84E-15	2.36E-13	5.83E-13	4.30E-13
298	3.30E-14	4.35E-13	1.04E-12	6.72E-13
400	1.04E-13	7.19E-13	1.69E-12	9.99E-13
500	2.33E-13	1.09E-12	2.52E-12	1.41E-12
600	4.35E-13	1.56E-12	3.57E-12	1.93E-12
700	7.23E-13	2.16E-12	4.85E-12	2.57E-12
800	1.11E-12	2.90E-12	6.38E-12	3.35E-12
900	1.42E-12	3.79E-12	8.18E-12	4.29E-12
1000	1.99E-12	4.85E-12	1.03E-11	5.39E-12
1100	2.68E-12	6.10E-12	1.27E-11	6.67E-12
1200	3.52E-12	7.54E-12	1.54E-11	8.15E-12
1300	4.52E-12	9.19E-12	1.84E-11	9.83E-12
1400	5.68E-12	1.11E-11	2.18E-11	1.17E-11
1500	7.01E-12	1.32E-11	2.56E-11	1.38E-11
1600	8.54E-12	1.55E-11	2.97E-11	1.62E-11
1800	1.22E-11	2.10E-11	3.92E-11	2.16E-11
2000	1.67E-11	2.76E-11	5.04E-11	2.81E-11
2200	2.22E-11	3.53E-11	6.33E-11	3.57E-11
2500	3.23E-11	4.93E-11	8.61E-11	4.94E-11
2800	4.49E-11	6.63E-11	1.13E-10	6.59E-11
3000	5.48E-11	7.94E-11	1.34E-10	7.86E-11

Table S5. Site-specific rate constants obtained with the MS-T-HL approach

T (K)	k (cm ³ molecule ⁻¹ s ⁻¹)			
	R1	R2	R3	R4
200	1.97E-14	1.61E-12	1.46E-12	3.51E-13
298	8.44E-14	2.15E-12	2.02E-12	3.82E-13
400	2.06E-13	2.85E-12	2.75E-12	4.50E-13
500	3.70E-13	3.66E-12	3.60E-12	5.43E-13
600	5.67E-13	4.58E-12	4.55E-12	6.60E-13
700	7.93E-13	5.63E-12	5.61E-12	8.03E-13
800	1.04E-12	6.80E-12	6.78E-12	9.72E-13
900	1.17E-12	8.10E-12	8.05E-12	1.17E-12
1000	1.45E-12	9.52E-12	9.43E-12	1.40E-12
1100	1.76E-12	1.11E-11	1.09E-11	1.65E-12
1200	2.09E-12	1.27E-11	1.25E-11	1.94E-12
1300	2.46E-12	1.45E-11	1.41E-11	2.26E-12
1400	2.85E-12	1.65E-11	1.59E-11	2.61E-12
1500	3.28E-12	1.85E-11	1.77E-11	2.99E-12
1600	3.74E-12	2.07E-11	1.96E-11	3.40E-12
1800	4.75E-12	2.53E-11	2.37E-11	4.32E-12
2000	5.90E-12	3.04E-11	2.81E-11	5.37E-12
2200	7.20E-12	3.59E-11	3.28E-11	6.54E-12
2500	9.42E-12	4.49E-11	4.02E-11	8.52E-12
2800	1.20E-11	5.47E-11	4.82E-11	1.08E-11
3000	1.39E-11	6.17E-11	5.37E-11	1.24E-11

Table S6. Site-specific rate constants obtained with the MS-T-HL_0.5 approach

T (K)	k (cm ³ molecule ⁻¹ s ⁻¹)			
	R1	R2	R3	R4
200	1.92E-14	1.53E-12	1.42E-12	3.25E-13
298	8.30E-14	2.09E-12	1.97E-12	3.63E-13
400	2.04E-13	2.80E-12	2.71E-12	4.34E-13
500	3.67E-13	3.61E-12	3.55E-12	5.28E-13
600	5.64E-13	4.54E-12	4.51E-12	6.45E-13
700	7.89E-13	5.59E-12	5.57E-12	7.87E-13
800	1.04E-12	6.76E-12	6.73E-12	9.56E-13
900	1.17E-12	8.06E-12	8.00E-12	1.15E-12
1000	1.45E-12	9.48E-12	9.37E-12	1.38E-12
1100	1.75E-12	1.10E-11	1.08E-11	1.63E-12
1200	2.09E-12	1.27E-11	1.24E-11	1.92E-12
1300	2.45E-12	1.45E-11	1.41E-11	2.24E-12
1400	2.85E-12	1.64E-11	1.58E-11	2.59E-12
1500	3.27E-12	1.85E-11	1.77E-11	2.96E-12
1600	3.73E-12	2.06E-11	1.96E-11	3.38E-12
1800	4.74E-12	2.53E-11	2.36E-11	4.29E-12
2000	5.90E-12	3.03E-11	2.80E-11	5.34E-12
2200	7.19E-12	3.58E-11	3.26E-11	6.50E-12
2500	9.41E-12	4.48E-11	4.01E-11	8.48E-12
2800	1.20E-11	5.46E-11	4.80E-11	1.07E-11
3000	1.39E-11	6.15E-11	5.36E-11	1.24E-11

Table S7. Site-specific rate constants obtained with the MS-T-HL_1.0 approach

T (K)	k (cm ³ molecule ⁻¹ s ⁻¹)			
	R1	R2	R3	R4
200	2.11E-14	1.58E-12	1.46E-12	3.22E-13
298	8.87E-14	2.14E-12	2.02E-12	3.53E-13
400	2.14E-13	2.86E-12	2.76E-12	4.22E-13
500	3.79E-13	3.67E-12	3.61E-12	5.13E-13
600	5.78E-13	4.60E-12	4.56E-12	6.29E-13
700	8.05E-13	5.65E-12	5.62E-12	7.69E-13
800	1.06E-12	6.82E-12	6.79E-12	9.36E-13
900	1.18E-12	8.12E-12	8.07E-12	1.13E-12
1000	1.46E-12	9.54E-12	9.44E-12	1.35E-12
1100	1.77E-12	1.11E-11	1.09E-11	1.61E-12
1200	2.11E-12	1.28E-11	1.25E-11	1.89E-12
1300	2.47E-12	1.46E-11	1.42E-11	2.20E-12
1400	2.87E-12	1.65E-11	1.59E-11	2.55E-12
1500	3.29E-12	1.85E-11	1.77E-11	2.92E-12
1600	3.75E-12	2.07E-11	1.97E-11	3.33E-12
1800	4.77E-12	2.53E-11	2.37E-11	4.24E-12
2000	5.92E-12	3.04E-11	2.81E-11	5.27E-12
2200	7.21E-12	3.59E-11	3.28E-11	6.43E-12
2500	9.44E-12	4.48E-11	4.02E-11	8.39E-12
2800	1.20E-11	5.46E-11	4.82E-11	1.06E-11
3000	1.39E-11	6.16E-11	5.37E-11	1.23E-11