Polycyclic Aromatic Hydrocarbon (PAH) Formation from Benzyl Radicals: A Reaction Kinetics Study

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Supplementary material

Table S1: *Rate constants for the elementary reactions. The units are cm, s, mol and cal.*

Reaction	A	n	E
Benzyl + Benzyl → IS1	4.53×10^{3}	2.450	-5829.4
IS1 → Benzyl + Benzyl	8.70×10^{09}	1.403	58325.5
IS1 + H → IS2 + H_2	1.63×10^{12}	0.699	17565.6
IS2 + H_2 → IS1 + H	1.82×10^{12}	0.323	6548.4
IS2 → IS3	8.15×10^{11}	-0.296	3786.7
IS3 → IS2	9.06×10^{11}	0.490	30714.2
IS3 → IS4 + H	1.27×10^{11}	0.676	26148.3
IS4 + H → IS3	9.13×10^{11}	0.424	10534.6
IS4 + H → IS5 + H_2	5.08×10^{11}	0.832	8432.6
IS5 + H_2 → IS4 + H	1.83×10^{13}	0.072	24917.6
IS4 → IS5 + H	8.15×10^{11}	1.058	104109.7
IS5 + H → IS4	9.06×10^{11}	0.359	15344.2
IS5 → Phenanthrene + H	1.26×10^{12}	0.486	30529.0
Phenanthrene + H → IS5	1.96×10^{11}	0.794	4075.3
IS4 → IS6 +H_2	1.26×10^{12}	0.852	97720.0
IS6 +H_2 → IS4	9.75×10^{10}	0.351	8508.9
IS6 → Phenanthrene	5.56×10^{11}	0.362	1025.4
Phenanthrene → IS6	1.09×10^{12}	0.572	79995.3
IS4 → Phenanthrene + H_2	5.57×10^{11}	0.773	104201.7
Phenanthrene + H_2 → IS4	5.47×10^{11}	0.248	94352.8
IS1 + H → IS7 + H_2	3.83×10^{12}	0.566	7604.9
IS7 + H_2 → IS1 + H	1.93×10^{12}	0.114	23852.6
IS1 → IS7 + H	5.08×10^{11}	1.171	107632.7
IS7 + H → IS1	9.13e11	0.301	19434.3
IS7 → IS2	1.92×10^{12}	0.225	65088.2
IS2 → IS7	9.65×10^{11}	0.313	37804.2
IS7 → IS8 + H	3.16×10^{11}	0.659	41314.9

IS8 + H → IS7	1.94×10^{12}	1.040	-308454.0
IS8 + H → IS9 + H_2	6.32×10^{11}	0.877	16666.7
IS9 + H_2 → IS8 + H	1.94×10^{12}	0.440	5889.5
IS9 → IS10	9.57×10^{11}	-0.149	3211.9
IS10 → IS9	4.85×10^{11}	0.567	36342.2
IS10 → Phenanthrene + H	8.00×10^{11}	0.453	19528.6
Phenanthrene + H → IS10	1.42×10^{11}	0.661	8723.2
IS8 + H → IS11 + H_2	1.91×10^{12}	0.448	16713.0
IS11 + H_2 → IS8 + H	9.70×10^{11}	0.168	18212.0
IS11 → IS12	4.22×10^{11}	0.296	49646.5
IS12 → IS11	9.16×10^{11}	0.399	11044.8
IS12 → IS13	7.92×10^{11}	-0.092	22740.6
IS13 → IS12	9.59×10^{11}	0.331	7676.2
IS13 → IS10	8.15×10^{11}	0.456	51041.3
IS10 → IS13	9.06×10^{11}	0.582	125405.1
IS9 → IS14	6.56×10^{11}	0.124	27455.4
IS14 → IS9	3.57×10^{11}	0.736	36175.4
IS14 → IS15	8.49×10^{11}	0.398	45006.9
IS15 → IS14	9.34×10^{11}	-0.047	12673.5
IS15 → IS16	6.79×10^{11}	-0.158	4161.9
IS16 → IS15	7.58×10^{11}	0.644	51282.9
IS16 → IS17 + H	7.43×10^{11}	0.461	16446.1
IS17 +H → IS16	3.92×10^{11}	0.535	9515.9
IS13 → IS18 + H_2	8.00×10^{11}	0.555	64369.0
IS18 + H_2 → IS13	1.42×10^{11}	0.588	120360.2
IS7 → IS19	6.55×10^{11}	-0.434	41750.9
IS19 → IS7	1.71×10^{11}	0.577	8154.6
IS19 → IS20 + H	7.06×10^{11}	0.575	27517.4
IS20 + H → IS19	3.18×10^{10}	0.696	7311.7
IS20 → IS21 + H	2.77×10^{11}	0.809	62412.2
IS21 + H → IS20	4.62×10^{10}	0.650	9710.6
IS21 → Phenanthrene + H	9.71×10^{10}	0.720	30135.8
Phenanthrene + H → IS21	8.23×10^{11}	0.527	4522.9
IS19 → IS22 + H	1.39×10^{12}	0.719	53940.0
IS22 + H → IS19	3.17×10^{11}	0.682	2970.9
IS22 → Phenanthrene + H_2	4.22×10^{11}	0.636	61205.9
Phenanthrene + H_2 → IS22	9.16×10^{11}	0.272	119089.0
IS20 → IS10 + H	1.90×10^{12}	0.708	74294.7
IS10 + H → IS20	3.44×10^{10}	0.543	386308.4
IS7 → IS23	4.39×10^{11}	-0.151	35709.0
IS23 → IS7	3.82×10^{11}	0.430	7238.4
IS23 → IS24	7.66×10^{11}	-0.141	59943.1
IS24 → IS23	7.95×10^{11}	0.365	4417.2

IS24 → IS25 + H	1.87×10^{11}	0.696	30508.1
IS25 + H → IS24	4.90×10^{11}	0.526	5328.3
IS25 → IS26 + H	4.46×10^{11}	0.835	57936.9
IS26 + H → IS25	6.46×10^{11}	0.237	5394.5
IS26 → IS27	7.09×10^{11}	0.518	28420.0
IS27 → IS26	7.55×10^{11}	0.132	24105.3
IS27 → IS28	2.76×10^{11}	0.541	35909.9
IS28 → IS27	6.80×10^{11}	0.498	72788.8
IS28 → IS29	6.55×10^{11}	0.352	54683.2
IS29 → IS28	1.63×10^{11}	0.663	12259.6
IS29 → IS30	1.19×10^{11}	0.743	46809.7
IS30 → IS29	4.98×10^{11}	0.535	47739.3
IS30 → IS10	9.60×10^{11}	0.319	2423.6
IS10 → IS30	3.40×10^{11}	0.453	52508.9
IS7 → IS31	5.85×10^{11}	0.130	51515.1
IS31 → IS7	2.24×10^{11}	0.473	2468.0
IS31 → IS32 + H	7.51×10^{11}	0.644	45493.6
IS32 + H → IS31	2.55×10^{11}	0.682	5016.5
IS32 + H → IS33 + H_2	7.92×10^{11}	0.690	19094.5
IS33 + H_2 → IS32 + H	9.59×10^{11}	0.337	9918.9
IS33 → IS34	5.06×10^{11}	-0.152	8102.6
IS34 → IS33	6.99×10^{11}	0.481	29679.4
IS34 → IS35	8.91×10^{11}	0.436	14940.7
IS35 → IS34	9.59×10^{11}	0.349	32916.7
IS35 → IS36	5.47×10^{11}	0.580	55329.5
IS36 → IS35	1.39×10^{11}	0.756	55790.3
IS36 → IS10	2.98×10^{11}	0.553	30384.1
IS10 → IS36	2.58×10^{11}	0.558	72635.4
IS1 → IS8 + H_2	1.31×10^{12}	0.479	107421.1
IS8 + H_2 → IS1	3.57×10^{10}	0.420	84986.1
IS1 → IS37 + H_2	1.69×10^{12}	0.723	100903.4
IS37 + H_2 → IS1	9.34×10^{11}	0.767	5226.6
IS37 → IS8	1.68×10^{12}	1.108	32165.3
IS8 → IS37	5.08×10^{11}	0.779	105786.9
IS37 → IS38	8.14×10^{11}	1.340	44517.2
IS38 → IS37	2.44×10^{11}	0.652	46541.0
IS38 → IS32	9.29×10^{11}	-0.018	16092.0
IS32 → IS38	3.50×10^{11}	0.540	36457.0
IS37 → IS39	1.97×10^{11}	1.088	22577.7
IS39 → IS37	2.51×10^{11}	0.651	16905.9
IS39 → IS40	6.16×10^{11}	-0.101	67988.9
IS40 → IS39	4.73×10^{11}	0.683	31237
IS40 → IS41	3.52×10^{11}	0.804	26751.4

IS41 → IS40	8.31×10^{11}	0.146	26334.2
IS41 → IS42	5.85×10^{11}	0.526	32907.2
IS42 → IS41	5.50×10^{11}	0.475	79236.8
IS42 → IS43	9.17×10^{11}	-0.0128	42386
IS43 → IS42	2.86×10^{11}	0.484	2441.7
IS43 → IS44	7.57×10^{11}	0.337	17552.7
IS44 → IS43	7.54×10^{11}	0.145	24310.9
IS44 → IS22	7.60×10^{11}	0.586	37179.0
IS22 → IS44	5.68×10^{11}	0.844	94701.1
IS37 → IS44	7.59×10^{11}	0.822	39618.7
IS44 → IS37	5.4×10^{10}	0.759	9933.0

Table S2: The energies (in hartree), molecular geometries (in Å), vibrational frequencies (in cm^{-1}), moments of inertia (in amu), and spin multiplicity of the intermediate species (IS) and the transition states (TS) before annihilation obtained using B3LYP/6-311++G(d,p).

Species	Energy (Ha)	Cartesian coordinate (Å)	Vibrational Frequencies (cm^{-1})	Moments of inertia (amu)	Multiplicity
IS1	-540.864183	C 0.3265 1.9202 0.0000 C 0.1614 2.6197 1.2010 C -0.1614 3.9756 1.2041 C -0.3253 4.6586 0.0000 C -0.1614 3.9756 -1.2041 C 0.1614 2.6197 -1.2010 H 0.2939 2.0983 2.1442 H -0.2800 4.4995 2.1463 H -0.5731 5.7140 0.0000 H -0.2800 4.4995 -2.1463 H 0.2939 2.0983 -2.1442 C 0.6377 0.4406 0.0000 H 1.2411 0.1874 0.8773 H 1.2411 0.1874 -0.8773 C -0.6377 -0.4406 0.0000 H -1.2411 -0.1874 -0.8773 H -1.2411 -0.1874 0.8773 C -0.3265 -1.9202 0.0000 C -0.1614 -2.6197 -1.2010 C -0.1614 -2.6197 1.2010 C 0.1614 -3.9756 -1.2041 H -0.2939 -2.0983 -2.1442 C 0.1614 -3.9756 1.2041 H -0.2939 -2.0983 2.1442 C 0.3253 -4.6586 0.0000 H 0.2800 -4.4995 -2.1463 H 0.2800 -4.4995 2.1463 H 0.5731 -5.7140 0.0000	22.0 37.3 54.1 61.4 119.2 235.2 291.5 315.3 372.2 413.1 413.6 479.9 532.6 534.5 625.0 635.5 636.7 711.6 711.7 752.8 769.8 771.0 803.5 853.5 853.6 860.4 921.2 923.4 980.0 980.3 996.3 996.9 997.1 1011.6 1016.9 1017.5 1049.4 1049.9 1087.8 1110.0 1163.2 1180.8 1181.5 1201.7 1202.0 1222.5 1223.1 1292.3 1295.4 1340.0 1341.1 1358.2 1361.0 1362.5 1481.8 1482.5 1486.9 1504.7 1525.4 1525.6 1622.0 1622.1 1642.9 1643.4 3024.7 3034.6 3055.6 3079.3 3150.1 3150.2 3151.1 3151.5 3165.1 3165.3 3173.8 3173.9 3186.5 3186.6	726.070 6757.459 7310.027	1
IS2	-540.179998	C -1.9223 0.0193 -0.3582 C -2.7216 1.1768 -0.3705 C -4.0868 1.1174 -0.0865 C -4.6991 -0.0970 0.2194 C -3.9336 -1.2731 0.2410 C -2.5979 -1.1431 -0.0458 H -2.2615 2.1306 -0.6133 H -4.6765 2.0270 -0.1076 H -5.7608 -0.1389 0.4376 H -4.3862 -2.2312 0.4723 C -0.4370 0.0616 -0.6379 H -0.1858 1.0051 -1.1310 H -0.1716 -0.7396 -1.3340 C 0.4174 -0.0871 0.6453 H 0.1531 -1.0301 1.1332 H 0.1510 0.7132 1.3425 C 1.9022 -0.0499 0.3630 C 2.5945 -1.2147 0.0112 C 2.6141 1.1538 0.4132 C 3.9558 -1.1787 -0.2844 H 2.0626 -2.1606 -0.0252 C 3.9760 1.1955 0.1186 H 2.0979 2.0671 0.6929 C 4.6517 0.0283 -0.2328 H 4.4742 -2.0936 -0.5500 H 4.5097 2.1384 0.1682 H 5.7116 0.0578 -0.4592	16.8 36.3 48.2 61.0 119.2 233.9 279.6 316.9 365.8 413.4 416.8 481.6 526.8 535.3 616.7 632.3 636.1 698.1 711.9 740.7 762.6 770.4 801.5 843.2 854.0 865.9 923.2 937.6 980.5 981.6 985.1 996.9 998.1 1012.3 1017.2 1042.2 1049.6 1091.3 1121.5 1164.5 1174.2 1181.2 1201.9 1215.4 1223.2 1263.3 1295.8 1308.4 1326.5 1341.2 1360.5 1363.4 1446.2 1472.1 1482.2 1486.3 1502.9 1525.5 1569.5 1622.0 1630.8 1643.2 3027.6 3037.9 3060.0 3083.6 3145.4 3150.5 3151.9 3159.1 3165.4 3171.7 3174.0 3184.2 3186.6	704.725 6796.922 7302.415	2

IS3	-540.223433	C	-1.3423	0.8202	-0.1703	47.9 84.3 148.6 197.4 259.1 308.9	1275.091	2
		C	-2.7098	0.8474	-0.4733	359.1 396.2 424.9 448.3 474.1 490.7	3248.107	
		C	-3.5026	-0.2884	-0.3611	525.8 538.2 597.5 603.7 665.8 679.5	4271.535	
		C	-2.9297	-1.4805	0.0789	723.7 747.3 761.0 778.7 796.1 833.1		
		C	-1.5736	-1.5197	0.3834	873.1 888.2 922.3 958.9 962.8 970.5		
		C	-0.7601	-0.3874	0.2501	976.4 991.2 1010.6 1029.3 1044.1		
		H	-3.1559	1.7834	-0.7960	1067.8 1125.9 1129.7 1171.0 1173.1		
		H	-4.5589	-0.2419	-0.6009	1184.6 1195.0 1201.0 1216.1 1225.3		
		H	-3.5356	-2.3728	0.1898	1232.0 1267.3 1306.6 1321.9 1337.0		
		H	-1.1442	-2.4499	0.7387	1347.8 1376.0 1404.7 1434.3 1477.7		
		C	-0.5284	2.0934	-0.2862	1479.6 1486.9 1519.6 1536.2 1606.0		
		H	-1.1591	2.9529	-0.0385	1614.7 1641.3 2812.1 2982.2 3009.2		
		H	-0.2053	2.2312	-1.3255	3050.8 3067.3 3143.3 3150.2 3154.9		
		C	0.7138	2.0634	0.6216	3160.9 3172.3 3184.4 3187.3 3193.3		
		H	0.3831	2.0894	1.6698			
		H	1.3362	2.9460	0.4527			
		C	1.4834	0.8086	0.3527			
		C	0.7348	-0.4779	0.6167			
		C	2.7613	0.7998	-0.1321			
		C	1.4361	-1.6832	0.0371			
		H	0.7376	-0.6141	1.7209			
		C	3.4202	-0.3976	-0.4978			
		H	3.2761	1.7470	-0.2685			
		C	2.7117	-1.6220	-0.4397			
		H	0.9135	-2.6317	0.0543			
		H	4.4351	-0.3690	-0.8743			
		H	3.1882	-2.5277	-0.8013			
IS4	-539.698260	C	1.4317	0.7984	0.2002	86.9 103.8 177.1 208.1 268.2 317.1	1181.913	1
		C	2.8267	0.8071	0.2001	392.1 396.8 456.3 467.3 469.9 504.2	3315.450	
		C	3.5536	-0.3618	-0.0141	554.0 577.9 611.8 635.9 721.5 738.4	4390.683	
		C	2.8771	-1.5582	-0.2443	740.2 758.0 783.6 791.2 818.4 879.3		
		C	1.4861	-1.5794	-0.2469	880.6 908.3 958.0 958.3 987.8 989.1		
		C	0.7417	-0.4140	-0.0124	991.2 1023.4 1049.5 1068.3 1069.7		
		H	3.3494	1.7441	0.3661	1110.8 1150.1 1181.1 1183.5 1187.5		
		H	4.6375	-0.3362	-0.0147	1208.6 1216.3 1224.1 1278.3 1303.8		
		H	3.4307	-2.4714	-0.4319	1306.0 1328.2 1334.8 1362.2 1380.6		
		H	0.9746	-2.5121	-0.4528	1470.9 1473.8 1483.2 1485.5 1516.4		
		C	0.6328	2.0603	0.4319	1521.2 1601.8 1622.3 1637.3 1645.9		
		H	1.2472	2.9392	0.2194	2989.0 3000.9 3064.8 3065.6 3153.2		
		H	0.3443	2.1216	1.4902	3153.5 3164.1 3166.3 3176.1 3180.9		
		C	-0.6328	2.0603	-0.4319	3187.4 3191.6		
		H	-0.3443	2.1216	-1.4902			
		H	-1.2472	2.9392	-0.2194			
		C	-1.4317	0.7984	-0.2002			
		C	-0.7417	-0.4140	0.0124			
		C	-2.8267	0.8071	-0.2001			
		C	-1.4861	-1.5794	0.2469			
		C	-3.5536	-0.3618	0.0141			
		H	-3.3494	1.7441	-0.3661			
		C	-2.8771	-1.5582	0.2443			
		H	-0.9746	-2.5121	0.4528			
		H	-4.6375	-0.3362	0.0147			
		H	-3.4307	-2.4714	0.4319			
IS5	-539.057512	C	1.4464	0.8609	0.0000	33.7 89.3 171.8 221.3 247.9 276.8	1161.950	2
		C	2.8735	0.8462	-0.0000	396.6 427.2 432.1 448.7 495.1 498.6	3315.357	
		C	3.5803	-0.3362	-0.0000	548.7 563.4 629.9 673.8 697.1 713.0	4466.447	
		C	2.8903	-1.5589	0.0000	717.5 730.3 761.4 782.4 818.6 851.7		
		C	1.4973	-1.5728	0.0000	863.2 865.3 927.7 941.5 962.4 973.9		
		C	0.7436	-0.3953	0.0000	987.4 1007.1 1041.4 1060.3 1074.4		
		H	3.3967	1.7968	-0.0000	1113.4 1153.7 1175.0 1187.6 1199.0		
		H	4.6645	-0.3233	-0.0000	1202.8 1216.7 1264.1 1296.6 1301.9		
		H	3.4375	-2.4943	0.0000	1329.4 1338.7 1375.7 1431.3 1447.2		
		H	0.9995	-2.5338	0.0000	1458.1 1483.2 1499.5 1532.8 1564.5		
		C	0.7509	2.0729	-0.0000	1603.2 1611.7 1641.7 2944.6 2947.1		
		H	1.3141	3.0006	-0.0000	3149.5 3156.3 3160.7 3166.8 3171.1		

		C	-0.7330	2.1613	0.0000	3180.8 3184.5 3192.5 3205.5		
		H	-1.0702	2.7501	-0.8685			
		H	-1.0702	2.7501	0.8685			
		C	-1.4445	0.8270	0.0000			
		C	-0.7342	-0.3920	0.0000			
		C	-2.8430	0.8165	0.0000			
		C	-1.4803	-1.5878	0.0000			
		C	-3.5600	-0.3724	0.0000			
		H	-3.3739	1.7639	0.0000			
		C	-2.8667	-1.5839	-0.0000			
		H	-0.9705	-2.5421	-0.0000			
		H	-4.6439	-0.3580	-0.0000			
		H	-3.4075	-2.5236	-0.0000			
IS6	-538.391340	C	-1.4402	0.8880	-0.0595	59.1 80.6 161.6 209.3 247.1 267.4	1132.901	1
		C	-2.8562	0.8814	-0.1038	400.3 419.6 440.2 448.1 487.9 500.1	3289.870	
		C	-3.5817	-0.2937	-0.0386	549.0 556.7 629.2 654.1 710.6 716.9	4406.002	
		C	-2.8886	-1.5049	0.0692	739.5 768.1 785.7 803.7 827.8 863.9		
		C	-1.4996	-1.5401	0.0980	878.8 895.9 961.9 992.7 996.0		
		C	-0.7410	-0.3617	0.0235	1013.1 1020.0 1038.4 1063.6 1069.1		
		H	-3.3419	1.8471	-0.1789	1113.3 1135.4 1151.9 1186.7 1189.2		
		H	-4.6649	-0.2828	-0.0646	1202.7 1250.3 1275.0 1286.6 1317.2		
		H	-3.4409	-2.4369	0.1306	1321.9 1339.1 1344.5 1374.8 1452.7		
		H	-1.0133	-2.5031	0.1859	1475.6 1496.0 1515.7 1578.9 1614.9		
		C	-0.8086	2.1800	-0.0933	1628.5 1642.4 2908.1 3020.3 3152.7		
		C	0.6542	2.1369	0.1015	3162.6 3168.7 3180.0 3182.7 3189.6		
		H	0.7174	2.5453	1.1328	3197.1 3203.4		
		H	1.1467	2.9256	-0.4815			
		C	1.4264	0.8448	0.0396			
		C	0.7320	-0.3798	0.0130			
		C	2.8247	0.8512	0.0144			
		C	1.4769	-1.5743	-0.0445			
		C	3.5449	-0.3344	-0.0364			
		H	3.3478	1.8026	0.0292			
		C	2.8625	-1.5542	-0.0661			
		H	0.9728	-2.5312	-0.0834			
		H	4.6287	-0.3146	-0.0595			
		H	3.4144	-2.4860	-0.1132			
IS7	-540.223632	C	-1.8755	0.1810	-0.0424	8.2 20.8 64.1 107.6 155.6 234.2	725.366	2
		C	-2.5396	-1.0655	0.1368	241.7 330.7 395.8 410.2 413.3 476.3	6996.635	
		C	-3.9235	-1.1401	0.1670	523.2 538.1 619.3 626.0 633.0 636.2	7085.973	
		C	-4.7039	0.0115	0.0216	686.3 712.7 762.6 763.5 816.0 827.6		
		C	-4.0750	1.2505	-0.1565	854.4 869.7 890.4 912.3 930.2 973.6		
		C	-2.6948	1.3374	-0.1884	980.2 985.3 993.2 997.5 1017.5		
		H	-1.9563	-1.9715	0.2509	1036.3 1049.7 1065.5 1097.5 1115.5		
		H	-4.4046	-2.1024	0.3047	1175.4 1176.0 1182.2 1187.7 1202.2		
		H	-5.7854	-0.0543	0.0463	1222.8 1237.0 1300.8 1335.2 1337.3		
		H	-4.6731	2.1481	-0.2701	1351.6 1358.3 1422.7 1470.01481.2		
		H	-2.2151	2.3008	-0.3267	1482.0 1504.7 1526.8 1577.6 1599.8		
		C	-0.4671	0.3005	-0.0791	1623.1 1643.9 2975.4 2994.0 3153.2		
		H	-0.0449	1.2894	-0.2249	3155.1 3155.8 3161.6 3163.1 3166.8		
		C	0.4931	-0.8475	0.0621	3173.3 3175.4 3182.4 3187.1 3190.3		
		H	0.3185	-1.5806	-0.7385			
		H	0.2912	-1.3886	0.9973			
		C	1.9451	-0.4189	0.0376			
		C	2.6654	-0.3947	-1.1607			
		C	2.5878	-0.0076	1.2101			
		C	3.9931	0.0302	-1.1892			
		H	2.1834	-0.7135	-2.0797			
		C	3.9149	0.4178	1.1867			
		H	2.0447	-0.0230	2.1499			
		C	4.6221	0.4388	-0.0145			
		H	4.5361	0.0390	-2.1279			
		H	4.3972	0.7295	2.1067			
		H	5.6553	0.7665	-0.0340			
IS8	-539.663737	C	-1.9385	-0.1858	0.0000	12.3 58.1 78.9 80.0 204.5 221.2	662.571	1

		C	-2.8265	-1.2754	0.0000	285.3 287.2 411.2 411.9 473.2 476.3	6890.463	
		C	-4.2057	-1.0868	-0.0000	542.1 551.6 632.5 636.1 655.1 699.4	7553.034	
		C	-4.7343	0.2018	0.0000	702.4 750.0 785.0 833.0 844.0 844.7		
		C	-3.8676	1.2973	0.0000	879.6 880.9 920.9 930.8 977.5 978.2		
		C	-2.4916	1.1081	0.0000	986.4 994.2 1002.5 1013.1 1014.0		
		H	-2.4236	-2.2832	0.0000	1048.2 1050.1 1102.3 1105.2 1181.9		
		H	-4.8665	-1.9465	-0.0000	1182.3 1204.0 1205.6 1211.0 1250.7		
		H	-5.8075	0.3542	-0.0000	1289.8 1328.9 1349.2 1355.3 1364.8		
		H	-4.2694	2.3046	0.0000	1371.1 1474.7 1482.9 1521.6 1530.0		
		H	-1.8423	1.9756	0.0000	1609.6 1615.1 1633.0 1642.0 1684.8		
		C	-0.4972	-0.4531	0.0000	3135.2 3144.0 3156.1 3156.1 3162.9		
		H	-0.2416	-1.5095	0.0000	3163.4 3172.9 3173.3 3182.3 3182.6		
		C	0.4972	0.4531	0.0000	3190.0 3190.3		
		H	0.2416	1.5095	0.0000			
		C	1.9385	0.1858	0.0000			
		C	2.8265	1.2754	0.0000			
		C	2.4916	-1.1081	0.0000			
		C	4.2057	1.0868	0.0000			
		H	2.4236	2.2832	0.0000			
		C	3.8676	-1.2973	0.0000			
		H	1.8423	-1.9756	0.0000			
		C	4.7343	-0.2018	-0.0000			
		H	4.8665	1.9465	-0.0000			
		H	4.2694	-2.3046	0.0000			
		H	5.8075	-0.3542	-0.0000			
IS9	-538.979693	C	1.9128	0.1766	0.0000	23.2 57.2 72.6 104.3 192.2 222.2	648.991	2
		C	2.7753	1.2863	0.0000	285.6 288.1 411.6 415.2 471.7 482.7	6859.730	
		C	4.1583	1.1283	0.0000	541.6 543.7 628.2 634.3 649.1 688.7	7508.721	
		C	4.7152	-0.1484	0.0000	702.9 739.2 772.0 832.3 841.4 846.2		
		C	3.8738	-1.2635	0.0000	880.9 886.4 926.1 935.7 975.1 979.1		
		C	2.4940	-1.1050	0.0000	984.9 990.7 1002.6 1013.7 1039.8		
		H	2.3490	2.2842	-0.0000	1049.1 1102.8 1117.0 1174.5 1182.2		
		H	4.8001	2.0023	-0.0000	1204.0 1210.1 1226.9 1258.2 1310.2		
		H	5.7916	-0.2767	0.0000	1325.7 1343.7 1354.6 1365.9 1445.5		
		H	4.2985	-2.2614	0.0000	1470.6 1479.4 1525.8 1562.8 1611.8		
		H	1.8634	-1.9863	0.0000	1621.3 1639.5 1682.2 3130.5 3147.0		
		C	0.4673	0.4099	0.0000	3151.2 3157.5 3160.2 3163.8 3172.4		
		H	0.1704	1.4565	0.0000	3173.6 3182.2 3186.0 3190.1		
		C	-0.5104	-0.5146	0.0000			
		H	-0.2592	-1.5715	0.0000			
		C	-1.9419	-0.2206	0.0000			
		C	-2.8970	-1.2612	-0.0000			
		C	-2.4884	1.0559	0.0000			
		C	-4.2646	-0.9930	0.0000			
		H	-2.5478	-2.2897	-0.0000			
		C	-3.8161	1.3839	0.0000			
		C	-4.7349	0.3192	0.0000			
		H	-4.9692	-1.8169	-0.0000			
		H	-4.1563	2.4139	0.0000			
		H	-5.7999	0.5239	0.0000			
IS10	-539.032829	C	-1.4413	0.9140	0.0870	49.0 93.5 205.0 211.6 247.9 373.9	1168.140	2
		C	-0.6871	2.1108	0.0464	388.2 414.3 429.0 485.0 487.0 519.1	3282.737	
		C	-1.5105	-1.6047	0.1399	543.9 565.0 602.6 665.6 687.5 716.3	4379.292	
		C	-2.8273	-1.5498	-0.1721	723.1 745.8 779.6 804.7 819.9 832.1		
		C	-3.5195	-0.3010	-0.2745	863.5 887.0 934.0 952.5 962.7 967.3		
		C	-2.8163	0.8882	-0.1718	976.7 986.0 1008.7 1045.9 1065.4		
		H	-1.2177	3.0517	-0.0654	1124.5 1132.4 1157.0 1181.9 1188.8		
		H	-1.0177	-2.5654	0.2135	1200.0 1215.9 1233.6 1248.8 1272.4		
		H	-3.3701	-2.4683	-0.3698	1306.8 1329.9 1335.9 1374.4 1419.1		
		H	-4.5790	-0.2913	-0.5003	1451.0 1476.4 1503.0 1518.2 1557.1		
		H	-3.3254	1.8315	-0.3470	1607.7 1622.1 1630.9 2767.0 3148.3		
		C	-0.7319	-0.3658	0.5004	3152.0 3157.3 3159.9 3168.5 3173.1		
		H	-0.7436	-0.3287	1.6161	3181.3 3187.3 3190.9 3202.0		
		C	0.6806	2.1019	0.0826			
		H	1.2319	3.0348	0.0330			

		C	1.4330	0.8666	0.0517			
		C	2.8262	0.8802	-0.1438			
		C	0.7608	-0.3759	0.1640			
		C	3.5491	-0.3011	-0.2327			
		H	3.3327	1.8360	-0.2326			
		C	1.5025	-1.5513	0.0677			
		C	2.8844	-1.5224	-0.1304			
		H	4.6223	-0.2731	-0.3838			
		H	1.0144	-2.5140	0.1515			
		H	3.4361	-2.4528	-0.2024			
IS11	-539.000180	C	1.9471	-0.4724	-0.0000	20.6 33.2 56.5 136.5 153.0 259.6	783.182	2
		C	3.1633	-1.1681	-0.0000	271.6 289.0 405.9 415.8 473.9 496.5	6640.831	
		C	4.3775	-0.4847	0.0000	523.1 533.3 613.2 625.7 634.1 676.5	6781.147	
		C	4.3953	0.9080	0.0000	704.3 746.4 751.4 771.9 820.2 826.4		
		C	3.1888	1.6120	0.0000	841.8 856.1 886.0 932.6 971.6 981.0		
		C	1.9779	0.9307	0.0000	982.7 984.8 999.6 1015.1 1030.1		
		H	3.1549	-2.2534	-0.0000	1047.3 1097.5 1100.2 1134.7 1172.9		
		H	5.3084	-1.0409	-0.0000	1181.1 1196.9 1200.9 1217.5 1289.7		
		H	5.3386	1.4423	0.0000	1299.5 1345.2 1349.2 1369.3 1451.3		
		H	3.1950	2.6965	0.0000	1477.6 1486.9 1522.8 1556.8 1586.0		
		H	1.0437	1.4817	0.0000	1617.9 1638.4 1865.5 3025.4 3155.6		
		C	0.6769	-1.2321	-0.0000	3161.3 3162.1 3167.7 3170.7 3177.9		
		H	0.7960	-2.3210	-0.0000	3184.7 3188.4 3189.2 3194.3		
		C	-0.5345	-0.7428	-0.0000			
		C	-1.8457	-0.3463	-0.0000			
		C	-2.5554	-0.1252	1.2258			
		C	-2.5554	-0.1252	-1.2258			
		C	-3.8755	0.2830	1.2110			
		H	-2.0373	-0.2856	2.1635			
		C	-3.8755	0.2830	-1.2110			
		H	-2.0373	-0.2856	-2.1635			
		C	-4.5497	0.4918	0.0000			
		H	-4.3939	0.4421	2.1503			
		H	-4.3939	0.4421	-2.1503			
		H	-5.5846	0.8124	0.0000			
IS12	-538.938968	C	-1.5801	-0.5540	0.0601	39.0 51.2 83.4 112.3 203.2 243.9	909.602	2
		C	-2.7177	-1.2685	-0.3718	306.2 316.2 386.7 412.0 485.8 505.9	5128.996	
		C	-3.9499	-0.6435	-0.5159	541.2 564.1 575.8 620.0 635.2 669.6	5660.951	
		C	-4.0846	0.7161	-0.2323	697.3 760.0 763.8 785.9 828.5 844.7		
		C	-2.9698	1.4408	0.1978	851.1 880.1 903.0 920.5 942.0 955.6		
		C	-1.7364	0.8206	0.3417	967.2 980.7 985.9 994.0 1006.0		
		H	-2.6211	-2.3263	-0.5938	1010.3 1045.4 1083.2 1105.2 1173.4		
		H	-4.8082	-1.2164	-0.8490	1180.1 1194.8 1201.4 1224.5 1275.2		
		H	-5.0452	1.2059	-0.3435	1311.1 1328.6 1353.2 1386.7 1428.5		
		H	-3.0671	2.4975	0.4223	1453.4 1485.2 1501.6 1518.3 1599.7		
		H	-0.8831	1.3951	0.6776	1604.7 1624.1 1665.4 3028.8 3129.2		
		C	-0.3186	-1.2538	0.1883	3138.5 3154.8 3156.8 3164.1 3165.9		
		H	-0.3372	-2.3202	-0.0258	3174.1 3179.8 3187.3 3203.1		
		C	0.8834	-0.7355	0.5675			
		C	2.2278	-0.8790	0.6978			
		C	1.6638	0.5111	0.9477			
		C	3.4297	-1.1295	-0.0201			
		C	2.1783	1.5016	-0.0223			
		H	1.5337	0.8654	1.9739			
		C	3.9201	-0.0874	-0.7533			
		H	3.9063	-2.1043	-0.0243			
		C	3.2348	1.1890	-0.8154			
		H	1.7863	2.5152	-0.0198			
		H	4.8208	-0.2186	-1.3432			
		H	3.6293	1.9384	-1.4938			
IS13	-538.914671	C	-1.5259	0.8516	0.3110	48.2 83.5 154.4 184.2 254.6 307.5	1255.243	2
		C	-2.9148	0.6142	0.0378	383.0 395.5 434.5 467.8 489.3 493.5	3104.228	
		C	-3.3142	-0.6051	-0.4254	536.0 559.4 589.2 638.5 664.1 690.2	3902.963	
		C	-2.3425	-1.6488	-0.6876	721.7 732.9 760.6 775.3 813.4 822.8		
		C	-1.0689	-1.5360	-0.2595	853.6 874.1 939.8 963.1 974.2 977.2		

		C	-0.6949	-0.3774	0.6315	980.6 987.7 995.1 1025.2 1043.8		
		H	-3.6066	1.4509	0.0558	1054.4 1127.0 1163.6 1167.5 1180.0		
		H	-4.3462	-0.7611	-0.7189	1201.0 1214.0 1243.8 1249.2 1284.3		
		H	-2.6540	-2.5167	-1.2589	1315.3 1334.1 1346.4 1389.2 1401.2		
		H	-0.3341	-2.3057	-0.4642	1416.7 1444.8 1462.1 1527.0 1555.4		
		H	-1.0381	-0.6884	1.6325	1600.7 1647.2 1674.3 2930.7 2990.9		
		C	-0.9245	2.0910	0.1738	3141.8 3145.9 3153.1 3161.8 3163.3		
		H	-1.5330	2.9897	0.1263	3170.9 3179.5 3187.9 3188.2		
		C	0.4512	2.1211	-0.0909			
		C	1.3182	1.0913	-0.0277			
		C	0.8398	-0.0369	0.8905			
		C	2.5118	0.9319	-0.8060			
		C	1.7345	-1.2431	0.8785			
		C	3.2303	-0.2200	-0.7593			
		H	2.8111	1.7483	-1.4538			
		C	2.8336	-1.3151	0.1076			
		H	1.4825	-2.0573	1.5523			
		H	4.1168	-0.3340	-1.3725			
		H	3.4613	-2.1996	0.1423			
		H	0.8371	0.3623	1.9121			
IS14	-538.994617	C	-1.3414	0.3530	-0.2557	23.3 62.1 82.7 205.2 231.9 262.6	964.550	2
		C	-2.4608	0.4875	-1.0820	318.6 393.8 414.5 441.8 489.3 519.2	4631.107	
		C	-3.7013	-0.0232	-0.6984	550.2 590.8 629.0 633.4 665.3 711.2	4743.666	
		C	-3.8382	-0.6779	0.5228	726.0 755.3 767.2 834.0 839.9 854.7		
		C	-2.7275	-0.8183	1.3566	865.6 906.6 927.0 940.6 952.4 979.8		
		C	-1.4918	-0.3075	0.9709	983.6 1000.3 1007.4 1016.8 1049.4		
		H	-2.3612	0.9975	-2.0352	1092.3 1102.0 1122.7 1158.6 1168.6		
		H	-4.5577	0.0917	-1.3538	1181.0 1186.4 1202.3 1217.6 1232.2		
		H	-4.8005	-1.0761	0.8244	1279.5 1310.6 1345.7 1365.4 1388.9		
		H	-2.8257	-1.3276	2.3091	1443.3 1482.8 1488.6 1524.5 1572.4		
		H	-0.6336	-0.4226	1.6242	1620.4 1628.2 1641.2 3024.6 3153.1		
		C	-0.0033	0.9171	-0.6792	3159.3 3160.1 3169.3 3169.9 3177.1		
		H	-0.1023	1.3849	-1.6651	3180.2 3186.9 3187.2 3210.1		
		C	0.7717	1.7962	0.3293			
		H	0.5197	2.7205	0.8315			
		C	1.8794	0.9100	0.3299			
		C	3.1668	0.6511	0.8322			
		C	1.2484	0.0171	-0.5766			
		C	3.7640	-0.5317	0.3939			
		H	3.6756	1.3149	1.5215			
		C	1.8328	-1.1500	-1.0030			
		C	3.1240	-1.4129	-0.4948			
		H	4.7564	-0.7870	0.7500			
		H	1.3520	-1.8414	-1.6861			
		H	3.6402	-2.3173	-0.7967			
IS15	-538.943279	C	1.4149	-0.4230	-0.0000	6.3 40.2 115.9 126.0 214.0 259.3	899.148	2
		C	1.7848	0.9363	-0.0001	287.5 317.2 409.5 414.6 453.9 479.4	4827.252	
		C	3.1211	1.3242	-0.0001	521.5 539.2 593.0 606.3 633.3 652.2	5726.400	
		C	4.1359	0.3703	0.0001	693.4 710.7 736.0 741.0 773.6 826.9		
		C	3.7991	-0.9859	0.0001	840.9 850.6 879.6 893.6 924.0 928.6		
		C	2.4683	-1.3716	0.0001	976.0 979.6 984.7 996.3 1011.7		
		H	1.0067	1.6955	-0.0002	1019.3 1048.5 1100.7 1131.9 1173.2		
		H	3.3690	2.3800	-0.0001	1181.6 1202.3 1210.4 1228.0 1246.3		
		H	5.1760	0.6763	0.0001	1333.4 1353.6 1396.2 1438.3 1454.9		
		H	4.5782	-1.7401	0.0002	1472.2 1491.1 1516.8 1562.9 1593.1		
		H	2.2202	-2.4280	0.0001	1609.5 1632.1 1667.7 3044.0 3125.3		
		C	0.0673	-0.9613	-0.0001	3157.0 3159.6 3165.3 3165.8 3175.6		
		H	0.0879	-2.0484	-0.0001	3180.6 3187.9 3189.7 3217.0		
		C	-0.9165	2.0347	-0.0000			
		H	-1.1173	3.0973	0.0000			
		C	-1.6932	0.9424	0.0000			
		C	-3.1443	1.1751	0.0001			
		C	-1.2216	-0.4688	-0.0001			
		C	-4.0402	0.1647	0.0001			
		H	-3.4771	2.2065	0.0002			

		C	-2.2660	-1.4838	-0.0001			
		C	-3.5898	-1.2025	-0.0000			
		H	-5.1031	0.3795	0.0002			
		H	-1.9411	-2.5187	-0.0002			
		H	-4.3179	-2.0054	-0.0000			
IS16	-539.018466	C	1.2125	0.7620	0.1780	74.9 91.6 202.6 219.4 243.7 344.1	885.955	2
		C	1.2486	-0.7290	0.4713	371.3 386.3 446.4 456.2 484.7 518.1	4017.883	
		C	2.4775	-1.4132	-0.0833	554.6 600.4 619.7 641.2 673.2 694.1	4835.243	
		C	3.5947	-0.7130	-0.3410	703.2 743.8 757.5 788.0 791.9 852.1		
		C	3.6216	0.7322	-0.1933	857.5 890.8 903.9 915.7 950.5 973.4		
		C	2.4792	1.4314	0.0311	975.9 983.3 984.6 1035.7 1051.0		
		H	1.3832	-0.7902	1.5814	1094.3 1137.4 1141.4 1168.7 1183.8		
		H	2.4469	-2.4915	-0.2003	1189.3 1205.2 1229.0 1265.1 1277.5		
		H	4.4904	-1.2173	-0.6876	1299.8 1347.0 1376.7 1396.0 1399.0		
		H	4.5593	1.2557	-0.3423	1436.5 1458.5 1500.4 1548.0 1559.8		
		H	2.4907	2.5171	0.0280	1608.5 1611.3 1671.6 2724.9 3142.9		
		C	0.0156	1.4094	0.0903	3152.2 3154.4 3156.3 3157.3 3160.6		
		H	0.0058	2.4902	-0.0243	3172.8 3174.2 3184.2 3188.0		
		C	-0.0455	-1.4202	0.1765			
		H	-0.0480	-2.5056	0.1550			
		C	-1.2455	-0.7254	0.0560			
		C	-2.5001	-1.3927	-0.0936			
		C	-1.2419	0.7201	0.0691			
		C	-3.6770	-0.6847	-0.1808			
		H	-2.5101	-2.4773	-0.1218			
		C	-2.4639	1.4070	-0.0233			
		C	-3.6666	0.7262	-0.1389			
		H	-4.6195	-1.2119	-0.2794			
		H	-2.4554	2.4923	-0.0121			
		H	-4.5982	1.2759	-0.2059			
IS17	-538.507730	C	1.2066	0.7273	-0.0780	90.3 119.5 235.4 235.9 266.5 386.8	839.387	1
		C	1.2016	-0.7155	-0.0974	395.6 397.5 477.0 485.1 506.5 535.1	3991.887	
		C	2.4541	-1.4034	-0.1251	589.5 616.8 641.4 660.8 740.0 756.7	4831.274	
		C	3.6352	-0.7144	-0.1332	762.8 769.8 783.3 820.1 841.4 863.5		
		C	3.6402	0.7104	-0.1140	898.7 910.3 918.3 928.8 970.9 977.0		
		C	2.4638	1.4070	-0.0873	992.1 992.2 1025.1 1029.6 1125.4		
		H	2.4498	-2.4884	-0.1397	1158.7 1172.4 1188.3 1189.7 1210.2		
		H	4.5778	-1.2497	-0.1543	1288.0 1290.1 1294.7 1337.2 1375.3		
		H	4.5864	1.2395	-0.1208	1413.2 1414.4 1426.4 1480.1 1484.4		
		H	2.4670	2.4920	-0.0727	1514.6 1576.6 1591.7 1620.7 1664.8		
		C	-0.0130	1.4118	-0.0508	1666.5 3153.2 3155.2 3156.9 3157.9		
		H	-0.0093	2.4976	-0.0362	3161.5 3163.0 3174.8 3175.1 3186.8		
		C	-0.0227	-1.3920	-0.0886	3187.2		
		H	-0.0265	-2.4778	-0.1032			
		C	-1.2423	-0.7075	-0.0614			
		C	-2.4996	-1.3872	-0.0521			
		C	-1.2373	0.7353	-0.0419			
		C	-3.6759	-0.6905	-0.0254			
		H	-2.5028	-2.4722	-0.0667			
		C	-2.4898	1.4232	-0.0142			
		C	-3.6710	0.7342	-0.0062			
		H	-4.6222	-1.2197	-0.0186			
		H	-2.4855	2.5082	0.0004			
		H	-4.6136	1.2696	0.0149			
IS18	-537.838002	C	1.4297	0.8835	-0.0000	48.2 83.5 154.4 184.2 254.6 307.5	1255.243	2
		C	2.8416	0.8725	-0.0000	383.0 395.5 434.5 467.8 489.3 493.5	3104.228	
		C	3.5420	-0.3156	0.0000	536.0 559.4 589.2 638.5 664.1 690.2	3902.963	
		C	2.8426	-1.5341	0.0000	721.7 732.9 760.6 775.3 813.4 822.8		
		C	1.4615	-1.5457	0.0000	853.6 874.1 939.8 963.1 974.2 977.2		
		C	0.7106	-0.3484	0.0000	980.6 987.7 995.1 1025.2 1043.8		
		H	3.3699	1.8201	0.0000	1054.4 1127.0 1163.6 1167.5 1180.0		
		H	4.6261	-0.3103	0.0000	1201.0 1214.0 1243.8 1249.2 1284.3		
		H	3.3881	-2.4709	0.0000	1315.3 1334.1 1346.4 1389.2 1401.2		
		H	0.9527	-2.5008	0.0000	1416.7 1444.8 1462.1 1527.0 1555.4		
		C	0.7045	2.1348	0.0000	1600.7 1647.2 1674.3 2930.7 2990.9		

		H	1.2570	3.0690	0.0000	3141.8 3145.9 3153.1 3161.8 3163.3		
		C	-0.6320	2.0777	0.0000	3170.9 3179.5 3187.9 3188.2		
		C	-1.4391	0.9176	-0.0000			
		C	-0.7485	-0.3370	0.0000			
		C	-2.8509	0.9548	-0.0000			
		C	-1.5361	-1.5094	0.0000			
		C	-3.5820	-0.2141	0.0000			
		H	-3.3445	1.9194	-0.0000			
		C	-2.9165	-1.4523	0.0000			
		H	-1.0579	-2.4805	-0.0000			
		H	-4.6653	-0.1802	0.0000			
		H	-3.4901	-2.3723	0.0000			
IS19	-540.171411	C	-1.5067	0.8165	0.2679	67.0 73.3 169.5 195.5 250.6 284.9	1368.989	2
		C	-0.9625	2.0269	0.0646	330.1 377.1 412.5 453.7 469.8 494.9	3030.505	
		C	-1.0317	-1.5676	-0.2325	506.0 550.7 585.0 632.6 649.2 685.5	3906.227	
		C	-2.2917	-1.7091	-0.6780	692.7 734.4 746.5 777.3 790.6 806.9		
		C	-3.2954	-0.6832	-0.4140	846.0 892.2 910.5 940.4 967.0 970.1		
		C	-2.9237	0.5395	0.0265	976.8 978.6 984.9 1007.5 1015.4		
		H	-1.6137	2.8705	-0.1530	1021.8 1055.2 1088.6 1127.7 1149.4		
		H	-0.2711	-2.3126	-0.4356	1173.7 1182.6 1186.4 1199.9 1204.2		
		H	-2.5771	-2.5787	-1.2606	1242.9 1257.5 1303.4 1317.7 1322.1		
		H	-4.3313	-0.8832	-0.6656	1361.7 1364.2 1393.5 1420.4 1434.3		
		H	-3.6401	1.3527	0.0899	1436.7 1461.2 1541.0 1584.5 1608.8		
		C	-0.6991	-0.4020	0.6742	1661.3 1693.1 2881.6 2911.3 2929.4		
		H	-1.0917	-0.6946	1.6653	3037.5 3132.6 3143.5 3146.4 3151.3		
		C	0.5233	2.2780	0.0306	3159.2 3164.6 3176.1 3184.8 3191.3		
		H	0.8212	2.8533	0.9249			
		C	1.3061	0.9986	-0.0289			
		C	2.3842	0.8017	-0.8445			
		C	0.8239	-0.0736	0.9107			
		C	3.1317	-0.4005	-0.8128			
		H	2.6881	1.5928	-1.5247			
		C	1.6994	-1.2928	0.9277			
		C	2.7761	-1.4238	0.1012			
		H	3.9821	-0.5290	-1.4709			
		H	1.4487	-2.0827	1.6292			
		H	3.3786	-2.3257	0.1450			
		H	0.7677	2.9181	-0.8240			
		H	0.8346	0.3679	1.9249			
IS20	-539.640194	C	-1.4546	0.8873	0.1486	18.8 94.6 182.8 201.0 248.6 283.4	1196.782	1
		C	-0.7936	2.0429	-0.0198	379.9 397.2 424.2 447.1 485.7 498.6	3318.544	
		C	-1.4563	-1.6127	-0.0963	528.2 554.2 603.0 671.8 679.6 696.4	4420.028	
		C	-2.7726	-1.5779	-0.3491	723.1 746.2 777.4 806.9 819.3 846.5		
		C	-3.5407	-0.3519	-0.1736	867.9 889.4 953.5 960.6 978.8 980.3		
		C	-2.9084	0.8201	0.0395	986.9 989.1 992.5 1035.5 1054.2		
		H	-1.3617	2.9538	-0.1921	1070.4 1132.1 1164.2 1185.4 1196.2		
		H	-0.8980	-2.5265	-0.2543	1204.6 1212.1 1218.4 1222.1 1268.5		
		H	-3.2812	-2.4635	-0.7151	1275.9 1296.6 1331.6 1373.6 1377.7		
		H	-4.6180	-0.3828	-0.2923	1401.5 1447.1 1465.9 1481.4 1523.6		
		H	-3.4630	1.7531	0.0625	1603.8 1616.2 1643.9 1676.7 1705.1		
		C	-0.7359	-0.4115	0.4921	2885.0 2959.1 3012.4 3136.6 3149.6		
		H	-0.8426	-0.5241	1.5888	3152.6 3160.3 3164.3 3175.9 3180.5		
		C	0.6948	2.1675	0.0167	3187.1 3197.5		
		H	0.9926	2.7144	0.9256			
		C	1.4276	0.8443	-0.0201			
		C	2.8074	0.8437	-0.2597			
		C	0.7674	-0.3703	0.2139			
		C	3.5446	-0.3333	-0.2460			
		H	3.3072	1.7882	-0.4535			
		C	1.5258	-1.5491	0.2454			
		C	2.8975	-1.5390	0.0195			
		H	4.6124	-0.3112	-0.4329			
		H	1.0433	-2.4952	0.4601			
		H	3.4571	-2.4672	0.0500			
		H	1.0330	2.8000	-0.8136			

IS21	-539.057512	C	-1.4464	0.8609	0.0000	33.7 89.3 171.8 221.3 247.9 276.9	1161.950	2
		C	-0.7509	2.0729	0.0000	396.6 427.2 432.1 448.7 495.1 498.6	3315.357	
		C	-1.4973	-1.5728	0.0000	548.7 563.4 629.9 673.8 697.1 713.0	4466.447	
		C	-2.8903	-1.5589	0.0000	717.5 730.3 761.4 782.4 818.6 851.7		
		C	-3.5803	-0.3362	0.0000	863.2 865.3 927.7 941.5 962.4 973.9		
		C	-2.8735	0.8462	-0.0000	987.4 1007.1 1041.4 1060.3 1074.4		
		H	-1.3141	3.0006	-0.0000	1113.4 1153.7 1175.0 1187.6 1199.0		
		H	-0.9995	-2.5338	0.0000	1202.8 1216.7 1264.1 1296.6 1301.9		
		H	-3.4375	-2.4943	0.0000	1329.4 1338.7 1375.7 1431.3 1447.2		
		H	-4.6645	-0.3233	-0.0000	1458.1 1483.2 1499.5 1532.8 1564.5		
		H	-3.3967	1.7968	-0.0000	1603.2 1611.7 1641.7 2944.6 2947.1		
		C	-0.7436	-0.3953	0.0000	3149.5 3156.3 3160.7 3166.8 3171.1		
		C	0.7330	2.1613	0.0000	3180.8 3184.5 3192.5 3205.5		
		H	1.0702	2.7501	0.8685			
		C	1.4445	0.8270	0.0000			
		C	2.8430	0.8165	0.0000			
		C	0.7342	-0.3920	0.0000			
		C	3.5600	-0.3724	0.0000			
		H	3.3739	1.7639	0.0000			
		C	1.4803	-1.5878	0.0000			
		C	2.8667	-1.5839	0.0000			
		H	4.6439	-0.3580	-0.0000			
		H	0.9705	-2.5421	0.0000			
		H	3.4075	-2.5236	-0.0000			
		H	1.0702	2.7501	-0.8685			
IS22	-539.590992	C	-1.3302	0.9916	-0.0477	76.6 88.7 158.2 194.5 257.9 326.7	1218.079	1
		C	-0.5166	2.0757	-0.1901	377.4 392.5 431.3 466.1 479.7 509.6	3232.523	
		C	-1.6470	-1.4208	0.6777	545.4 560.7 589.5 646.2 685.5 700.1	4100.411	
		C	-2.8603	-1.4162	0.0995	712.0 736.6 762.6 784.0 817.0 825.0		
		C	-3.3966	-0.2153	-0.5165	864.2 899.4 924.9 947.5 967.2 976.7		
		C	-2.6618	0.9244	-0.5811	979.8 982.8 984.9 994.8 1025.8		
		H	-0.8983	2.9817	-0.6503	1067.4 1094.8 1107.5 1163.6 1175.6		
		H	-1.2646	-2.3219	1.1477	1180.4 1202.4 1212.3 1244.6 1263.8		
		H	-3.4622	-2.3188	0.0875	1270.9 1311.7 1334.8 1369.5 1386.3		
		H	-4.3879	-0.2504	-0.9540	1396.3 1408.4 1440.2 1458.4 1522.4		
		H	-3.0547	1.8026	-1.0846	1563.4 1592.1 1634.6 1660.1 1682.6		
		C	-0.8014	-0.1810	0.7637	2914.3 2943.0 3144.5 3147.6 3151.8		
		H	-0.8649	0.1666	1.8084	3153.2 3159.4 3162.6 3168.4 3178.8		
		C	0.8818	2.0144	0.1399	3183.7 3187.1		
		H	1.4816	2.9124	0.0216			
		C	1.5134	0.8295	0.3745			
		C	2.9436	0.6600	0.2142			
		C	0.7334	-0.4531	0.5757			
		C	3.4228	-0.5012	-0.3010			
		H	3.6006	1.5090	0.3774			
		C	1.2018	-1.5048	-0.4096			
		C	2.5048	-1.5407	-0.7450			
		H	4.4826	-0.6141	-0.4999			
		H	0.5090	-2.2619	-0.7576			
		H	2.8876	-2.3333	-1.3794			
		H	1.0453	-0.8467	1.5573			
IS23	-540.178942	C	1.3841	-0.0820	0.2760	34.4 63.1 77.2 177.5 214.3 239.0	897.502	2
		C	1.9632	-0.7086	-0.8360	310.0 361.2 403.4 413.9 490.6 529.4	4972.738	
		C	3.3144	-0.5431	-1.1295	551.2 562.7 585.1 634.2 666.0 685.9	5258.790	
		C	4.1181	0.2542	-0.3148	711.2 754.5 758.2 767.2 825.3 852.1		
		C	3.5575	0.8834	0.7942	866.2 897.6 912.0 938.6 963.3 965.2		
		C	2.2042	0.7151	1.0838	979.2 982.5 995.2 999.8 1016.3		
		H	1.3565	-1.3342	-1.4824	1035.7 1050.9 1079.2 1102.9 1122.3		
		H	3.7412	-1.0381	-1.9949	1137.8 1161.8 1181.6 1200.8 1205.4		
		H	5.1702	0.3819	-0.5428	1209.3 1224.6 1226.1 1285.8 1310.1		
		H	4.1723	1.5050	1.4359	1338.1 1350.1 1382.0 1390.9 1425.9		
		H	1.7761	1.2087	1.9506	1474.3 1483.9 1525.5 1528.6 1617.3		
		C	-0.0771	-0.2318	0.5997	1621.5 1641.4 2908.3 3027.2 3070.3		
		H	-0.3053	0.2791	1.5370	3087.4 3147.3 3149.7 3153.9 3156.9		
		C	-0.7564	-1.6558	0.6201	3167.7 3167.9 3175.7 3187.4 3187.7		

		H	-0.8685	-2.1414	1.5919			
		H	-0.2513	-2.3457	-0.0641			
		C	-1.9668	-0.9854	0.0193			
		C	-3.3073	-0.9523	0.2373			
		C	-1.1761	0.1867	-0.4814			
		C	-4.0095	0.2498	-0.0610			
		H	-3.8276	-1.7822	0.7068			
		C	-1.9328	1.4693	-0.5216			
		H	-0.7251	-0.0199	-1.4681			
		C	-3.2947	1.4399	-0.3701			
		H	-5.0861	0.2903	0.0519			
		H	-1.4178	2.3972	-0.7481			
		H	-3.8577	2.3629	-0.4699			
IS24	-540.090471	C	1.0281	0.7454	-0.3998	84.4 103.3 202.8 227.3 249.9 348.6	1143.305	2
		C	2.2214	1.3777	-0.2391	355.2 404.2 456.0 485.7 512.7 517.0	3125.810	
		C	3.4040	0.6293	0.0046	550.1 573.6 614.8 648.8 668.7 675.7	4038.356	
		C	3.3376	-0.7759	0.1769	736.6 766.1 772.3 813.0 848.5 862.7		
		C	2.1687	-1.4707	0.0296	888.0 905.1 913.7 937.9 949.8 962.8		
		C	0.9014	-0.7975	-0.3875	978.8 987.1 991.8 997.5 1019.3		
		H	2.2683	2.4622	-0.2522	1031.8 1053.3 1076.6 1122.1 1132.7		
		H	4.3513	1.1420	0.1195	1153.8 1169.5 1182.7 1183.4 1202.9		
		H	4.2432	-1.3115	0.4435	1207.5 1243.9 1267.0 1294.2 1319.0		
		H	2.1539	-2.5477	0.1674	1333.0 1346.1 1374.4 1405.1 1421.4		
		H	0.6611	-1.1219	-1.4166	1426.1 1452.2 1485.7 1537.0 1595.3		
		C	-0.4082	1.1701	-0.3839	1612.8 1680.2 2893.3 2994.7 3022.9		
		H	-0.8377	0.7226	-1.2885	3041.4 3060.0 3128.3 3133.1 3146.0		
		C	-1.5247	2.2092	0.0523	3149.5 3154.5 3161.2 3164.9 3188.9		
		H	-1.9890	2.8093	-0.7293			
		H	-1.2359	2.8327	0.9011			
		C	-2.2205	0.8845	0.4725			
		C	-3.1497	0.1022	-0.0987			
		C	-0.8899	0.2907	0.7977			
		C	-2.8297	-1.3273	-0.2831			
		H	-4.0202	0.5036	-0.6084			
		C	-0.4333	-1.1182	0.4934			
		H	-0.4640	0.7060	1.7159			
		C	-1.5965	-1.8640	-0.1309			
		H	-3.6174	-1.9623	-0.6785			
		H	-0.1172	-1.6586	1.3912			
		H	-1.4494	-2.9093	-0.3899			
IS25	-539.550246	C	1.0229	0.7510	-0.0735	104.0 129.0 217.8 250.1 268.6 361.9	1133.299	1
		C	2.2268	1.3723	-0.3598	398.7 403.4 475.7 492.8 506.7 549.6	3125.613	
		C	3.4055	0.6128	-0.3515	566.9 606.4 650.0 683.0 715.2 746.1	3961.929	
		C	3.3667	-0.7505	-0.0770	755.8 777.2 828.3 845.2 861.1 888.6		
		C	2.1501	-1.3836	0.2136	900.9 929.1 952.4 954.4 981.8 986.6		
		C	0.9772	-0.6446	0.2215	990.9 994.4 1015.2 1033.1 1042.9		
		H	2.2607	2.4310	-0.5929	1075.9 1099.1 1138.6 1157.1 1163.6		
		H	4.3540	1.0929	-0.5658	1178.5 1181.6 1191.1 1206.9 1254.5		
		H	4.2857	-1.3262	-0.0745	1273.8 1307.9 1318.2 1333.6 1343.6		
		H	2.1352	-2.4432	0.4499	1404.1 1425.3 1449.7 1464.8 1484.1		
		C	-0.4390	1.1671	-0.1675	1487.5 1588.0 1610.9 1638.3 1672.3		
		H	-0.7256	0.7529	-1.1408	3001.2 3005.0 3035.2 3060.8 3130.6		
		C	-1.6529	2.1584	0.1182	3137.0 3151.4 3153.4 3162.0 3162.7		
		H	-2.0164	2.7651	-0.7101	3173.3 3184.8		
		H	-1.5305	2.7604	1.0208			
		C	-2.3427	0.7842	0.3786			
		C	-3.0943	-0.0200	-0.3926			
		C	-1.0536	0.2523	0.9040			
		C	-2.6200	-1.4001	-0.6174			
		H	-3.8838	0.3577	-1.0352			
		C	-0.4507	-1.1122	0.6551			
		H	-0.7966	0.6671	1.8840			
		C	-1.3921	-1.8609	-0.2819			
		H	-3.2574	-2.0461	-1.2146			
		H	-0.3489	-1.7136	1.5666			

		H	-1.0989	-2.8552	-0.6057			
IS26	-538.967171	C	0.8594	0.7997	0.2903	89.5 103.0 207.3 208.8 305.5 346.1	1372.856	2
		C	2.0276	1.3521	-0.2559	396.0 445.6 483.0 500.3 515.4 543.5	2575.805	
		C	3.0948	0.5141	-0.5655	548.5 601.2 621.6 681.6 713.7 736.6	3312.157	
		C	3.0034	-0.8649	-0.3508	749.0 766.1 799.1 824.5 844.0 871.9		
		C	1.8317	-1.4277	0.1680	910.4 942.1 951.8 954.4 972.1 982.1		
		C	0.7655	-0.6032	0.4939	984.6 993.2 1026.4 1042.3 1068.2		
		H	2.1011	2.4217	-0.4193	1091.2 1107.7 1128.4 1149.9 1166.7		
		H	4.0069	0.9332	-0.9760	1182.8 1192.2 1201.0 1235.9 1285.3		
		H	3.8449	-1.5037	-0.5946	1295.9 1300.4 1321.6 1343.9 1360.5		
		H	1.7615	-2.5022	0.3033	1406.5 1468.0 1480.5 1484.4 1579.1		
		C	-0.3633	1.4457	0.7000	1595.4 1615.5 1666.7 3026.5 3036.0		
		C	-1.3877	2.2164	-0.1382	3050.2 3092.4 3146.7 3156.5 3160.3		
		H	-1.0608	2.6538	-1.0834	3163.7 3171.7 3174.8 3186.2		
		H	-1.9612	2.9467	0.4408			
		C	-1.9956	0.8191	-0.1786			
		C	-2.2884	-0.0427	-1.1714			
		C	-1.3417	0.3560	1.1179			
		C	-2.1602	-1.4765	-0.9104			
		H	-2.5465	0.3004	-2.1681			
		C	-0.6229	-1.0010	1.0171			
		H	-1.9267	0.5306	2.0246			
		C	-1.3826	-1.9409	0.0853			
		H	-2.6614	-2.1755	-1.5727			
		H	-0.5321	-1.4723	2.0003			
		H	-1.2659	-3.0095	0.2344			
IS27	-538.960610	C	1.0197	0.7004	0.0220	42.6 95.8 129.0 176.8 246.2 277.6	1310.058	2
		C	2.3012	1.1031	-0.3658	370.3 389.2 418.5 458.5 474.4 529.2	2983.101	
		C	3.3239	0.1606	-0.4176	535.2 568.1 596.8 623.4 674.8 689.2	3961.923	
		C	3.0773	-1.1740	-0.0794	718.8 751.4 774.0 800.6 820.6 831.4		
		C	1.8004	-1.5787	0.3103	873.9 891.3 908.1 924.4 935.8 952.9		
		C	0.7758	-0.6377	0.3568	961.6 972.0 991.3 1007.2 1046.6		
		H	2.5020	2.1389	-0.6159	1048.9 1109.0 1129.3 1173.5 1182.5		
		H	4.3216	0.4639	-0.7144	1202.8 1215.9 1246.9 1258.3 1276.2		
		H	3.8847	-1.8967	-0.1160	1305.8 1314.4 1327.5 1351.1 1392.2		
		H	1.6148	-2.6146	0.5750	1440.8 1489.1 1500.6 1616.2 1635.1		
		C	-0.2049	1.5035	0.1583	1639.1 1695.7 1705.6 2991.5 3014.1		
		C	-0.4065	2.7618	-0.2389	3138.6 3145.9 3155.7 3157.7 3165.6		
		H	0.3744	3.3373	-0.7230	3171.5 3176.4 3187.6 3220.2		
		H	-1.3642	3.2498	-0.1019			
		C	-2.6166	0.7242	0.3341			
		C	-3.2868	-0.1266	-0.4199			
		C	-1.2421	0.6116	0.8598			
		C	-2.6112	-1.3866	-0.7985			
		H	-4.2930	0.0663	-0.7781			
		C	-0.6810	-0.8677	0.7254			
		H	-1.2264	0.8716	1.9250			
		C	-1.4187	-1.7182	-0.2903			
		H	-3.1100	-2.0422	-1.5053			
		H	-0.7432	-1.3784	1.6951			
		H	-0.9422	-2.6501	-0.5785			
IS28	-539.019405	C	1.1570	0.6621	0.0243	74.5 111.7 135.9 200.8 243.2 272.5	1312.129	2
		C	2.5010	0.9614	-0.2002	378.2 394.1 419.0 438.6 497.4 519.4	3064.490	
		C	3.4266	-0.0789	-0.2628	547.2 589.5 605.3 620.3 634.3 694.0	4294.216	
		C	3.0186	-1.4050	-0.0955	701.1 731.3 764.9 776.7 788.6 817.0		
		C	1.6765	-1.7080	0.1460	843.2 845.8 884.6 926.3 955.4 960.2		
		C	0.7526	-0.6724	0.1988	971.3 988.0 991.6 1038.5 1043.8		
		H	2.8266	1.9870	-0.3349	1076.9 1120.8 1130.4 1153.6 1170.9		
		H	4.4722	0.1417	-0.4464	1184.7 1198.7 1219.9 1245.9 1274.3		
		H	3.7496	-2.2038	-0.1521	1296.4 1336.1 1353.5 1384.1 1423.8		
		H	1.3686	-2.7388	0.2865	1430.6 1492.3 1494.9 1514.0 1586.4		
		C	-0.0168	1.5662	0.0957	1612.4 1620.1 1644.5 2816.6 3146.4		
		C	0.0044	2.9199	0.0408	3154.5 3157.8 3158.7 3165.5 3174.8		
		H	0.9314	3.4691	-0.0677	3176.1 3187.1 3188.4 3230.0		
		H	-0.9050	3.5042	0.1089			

		C	-2.5156	0.9682	-0.0314			
		C	-3.4113	-0.0852	-0.2246			
		C	-1.1777	0.7034	0.2138			
		C	-2.9399	-1.4365	-0.3117			
		H	-4.4538	0.1249	-0.4319			
		C	-0.7306	-0.7116	0.5143			
		C	-1.6479	-1.7589	-0.0462			
		H	-3.6326	-2.2067	-0.6348			
		H	-0.7898	-0.8350	1.6191			
		H	-1.2938	-2.7799	-0.1388			
		H	-2.8544	1.9893	-0.1759			
IS29	-538.951879	C	-1.1252	0.7857	0.2588	74.6 95.2 170.1 214.3 253.9 353.9	1195.638	2
		C	-2.4290	1.0813	0.6587	377.2 402.2 435.1 463.0 471.2 527.6	3099.237	
		C	-3.4149	0.1040	0.5237	567.7 584.9 612.0 644.5 709.6 731.6	3914.596	
		C	-3.1082	-1.1423	-0.0267	742.3 769.2 784.3 796.4 809.4 862.9		
		C	-1.8075	-1.4315	-0.4508	888.6 896.5 946.0 956.7 969.6 976.8		
		C	-0.8142	-0.4739	-0.2915	988.6 990.1 1011.3 1021.3 1035.8		
		H	-2.6666	2.0528	1.0770	1044.4 1049.2 1122.2 1167.6 1176.9		
		H	-4.4289	0.3145	0.8447	1187.6 1195.7 1205.1 1230.1 1268.7		
		H	-3.8851	-1.8920	-0.1270	1290.4 1309.6 1330.2 1360.8 1401.7		
		H	-1.5839	-2.3979	-0.8912	1444.0 1464.9 1481.8 1485.4 1606.1		
		C	0.0718	1.6239	0.2745	1627.1 1631.6 1695.3 2936.9 3073.9		
		C	0.7217	2.1186	-0.9509	3149.1 3156.2 3157.5 3160.3 3166.4		
		H	0.1866	2.0500	-1.8966	3170.0 3178.1 3182.4 3188.2		
		H	1.4159	2.9519	-0.8860			
		C	2.5795	0.8472	0.3441			
		C	3.2249	-0.2879	0.6552			
		C	1.2302	0.8238	-0.2533			
		C	2.6107	-1.5951	0.4252			
		H	4.2089	-0.2486	1.1088			
		C	0.6545	-0.5398	-0.7141			
		C	1.4249	-1.7248	-0.1841			
		H	3.1405	-2.4783	0.7667			
		H	0.6806	-0.5961	-1.8154			
		H	0.9934	-2.7076	-0.3454			
		H	3.0233	1.8154	0.5518			
IS30	-538.953143	C	-1.0986	0.7927	0.2305	76.0 98.8 171.1 211.2 262.1 351.3	1176.630	2
		C	-2.3867	1.0706	0.6831	378.7 396.0 444.2 464.2 478.6 537.4	3088.062	
		C	-3.3786	0.0965	0.5544	552.2 584.9 611.5 665.3 671.2 718.6	3833.974	
		C	-3.0872	-1.1350	-0.0328	727.5 746.4 772.3 780.8 808.1 849.7		
		C	-1.7956	-1.4118	-0.4897	867.6 897.5 931.5 952.2 959.2 972.9		
		C	-0.8013	-0.4505	-0.3495	982.3 988.3 989.4 992.4 1038.2		
		H	-2.6179	2.0320	1.1289	1046.8 1057.1 1118.5 1154.7 1178.7		
		H	-4.3826	0.3004	0.9097	1180.1 1196.9 1200.2 1229.4 1235.9		
		H	-3.8653	-1.8835	-0.1316	1254.9 1302.1 1307.9 1333.1 1355.9		
		H	-1.5756	-2.3747	-0.9394	1400.2 1442.3 1484.2 1499.3 1614.3		
		C	0.0999	1.6793	0.2457	1627.0 1635.0 1694.4 2957.4 3127.8		
		C	0.6626	1.9730	-1.0826	3147.6 3156.6 3159.9 3163.5 3166.8		
		H	0.1823	2.0491	-2.0516	3169.9 3174.4 3183.1 3186.6		
		C	2.6216	0.8804	0.1874			
		C	3.2344	-0.2301	0.6266			
		C	1.2593	0.8232	-0.3873			
		C	2.5802	-1.5361	0.5508			
		H	4.2271	-0.1707	1.0587			
		C	0.6710	-0.5687	-0.7417			
		C	1.3997	-1.7042	-0.0598			
		H	3.0796	-2.3871	1.0025			
		H	0.7336	-0.7358	-1.8284			
		H	0.9421	-2.6873	-0.1121			
		H	3.0978	1.8523	0.2591			
		H	0.2952	2.3300	1.0934			
IS31	-540.146297	C	-1.5991	-0.1170	-1.1805	20.8 41.1 66.0 78.9 151.9 236.1	1006.338	2
		C	-1.8637	1.2431	-0.8980	277.7 351.0 394.8 414.2 478.6 519.9	4655.866	
		C	-2.8535	1.5743	-0.0050	525.5 537.5 574.9 625.4 636.1 666.3	5181.630	
		C	-3.5320	0.5445	0.7466	712.2 744.2 769.0 787.9 820.7 852.9		

		C	-3.3009	-0.7754	0.5295	854.7 856.1 908.9 925.7 930.5 941.1		
		C	-2.3605	-1.2093	-0.5183	974.2 982.5 989.8 993.8 998.8		
		H	-1.2675	2.0197	-1.3697	1017.3 1049.6 1051.8 1068.6 1100.4		
		H	-3.0965	2.6136	0.1868	1121.9 1172.3 1180.7 1193.5 1202.0		
		H	-4.2635	0.8455	1.4895	1203.0 1219.9 1307.4 1318.4 1334.2		
		H	-3.8886	-1.5240	1.0526	1345.2 1360.4 1392.2 1427.6 1435.3		
		H	-2.6893	-2.0654	-1.1076	1482.4 1485.9 1505.8 1525.4 1620.4		
		C	-0.7820	-1.1342	-0.5118	1622.4 1642.8 3018.6 3066.8 3076.7		
		H	-0.3635	-1.9275	-1.1284	3098.8 3138.5 3145.7 3149.8 3157.1		
		C	0.0203	-0.8314	0.7457	3165.3 3167.2 3174.9 3179.0 3186.6		
		H	0.0828	-1.7475	1.3446			
		H	-0.5162	-0.0929	1.3462			
		C	1.4180	-0.3322	0.4405			
		C	2.4489	-1.2321	0.1449			
		C	1.7071	1.0365	0.4230			
		C	3.7291	-0.7792	-0.1666			
		H	2.2487	-2.2992	0.1651			
		C	2.9868	1.4945	0.1129			
		H	0.9235	1.7486	0.6599			
		C	4.0023	0.5880	-0.1853			
		H	4.5144	-1.4933	-0.3894			
		H	3.1914	2.5597	0.1087			
		H	4.9987	0.9425	-0.4240			
IS32	-539.582447	C	-1.5927	0.2626	-0.4235	24.9 32.7 65.7 105.4 172.7 248.7	868.313	1
		C	-2.2823	1.4543	-0.4979	327.6 346.3 394.4 413.6 446.8 510.5	5441.490	
		C	-3.6553	1.3301	-0.2036	519.5 572.4 626.9 636.0 681.7 711.9	6003.289	
		C	-4.2374	0.1018	0.1391	726.5 748.3 758.2 815.5 853.6 855.1		
		C	-3.4879	-1.0901	0.2111	895.7 928.9 936.7 966.0 981.4 991.3		
		C	-2.1538	-0.9219	-0.0947	998.1 1006.5 1017.0 1018.2 1030.9		
		H	-1.8443	2.4119	-0.7562	1049.8 1082.2 1103.5 1124.6 1136.0		
		H	-4.2863	2.2118	-0.2418	1176.6 1180.7 1195.5 1202.2 1221.1		
		H	-5.2999	0.0721	0.3559	1296.7 1314.6 1337.3 1353.8 1366.0		
		H	-3.9512	-2.0318	0.4836	1384.6 1471.2 1477.7 1482.6 1487.6		
		C	-0.6753	-0.9269	-0.3752	1525.5 1602.6 1622.4 1643.0 1724.9		
		H	-0.3466	-1.3406	-1.3312	3028.4 3050.7 3077.6 3151.0 3155.9		
		C	0.3618	-1.1151	0.7371	3156.1 3165.5 3166.6 3174.2 3174.9		
		H	0.5011	-2.1899	0.8950	3183.1 3186.8		
		H	-0.0385	-0.7017	1.6667			
		C	1.6894	-0.4702	0.4050			
		C	2.6765	-1.1763	-0.2915			
		C	1.9461	0.8604	0.7550			
		C	3.8851	-0.5713	-0.6327			
		H	2.5004	-2.2126	-0.5634			
		C	3.1534	1.4690	0.4175			
		H	1.1945	1.4223	1.3002			
		C	4.1271	0.7551	-0.2794			
		H	4.6389	-1.1372	-1.1690			
		H	3.3354	2.4996	0.7022			
		H	5.0681	1.2265	-0.5400			
IS33	-538.901254	C	-1.5715	0.2456	-0.4369	22.9 31.1 64.6 107.1 168.8 244.9	857.161	2
		C	-2.2441	1.4436	-0.5542	327.0 346.1 385.7 417.3 448.0 510.5	5485.261	
		C	-3.6182	1.3498	-0.2541	515.1 569.7 618.9 632.3 680.0 696.9	5940.576	
		C	-4.2174	0.1432	0.1336	726.2 740.3 750.6 814.6 835.0 867.9		
		C	-3.4853	-1.0560	0.2480	895.8 935.0 940.1 962.8 978.5 989.6		
		C	-2.1494	-0.9179	-0.0648	991.0 1006.0 1018.0 1028.0 1044.0		
		H	-1.7928	2.3848	-0.8474	1084.6 1119.8 1124.9 1136.8 1172.6		
		H	-4.2366	2.2385	-0.3237	1176.6 1188.5 1214.5 1284.1 1297.1		
		H	-5.2800	0.1368	0.3520	1313.7 1322.8 1360.9 1384.4 1446.8		
		H	-3.9616	-1.9806	0.5546	1471.0 1473.2 1477.8 1485.2 1569.9		
		C	-0.6727	-0.9555	-0.3479	1602.7 1630.9 1725.3 3034.6 3055.8		
		H	-0.3483	-1.4096	-1.2865	3084.9 3149.4 3156.3 3159.7 3165.9		
		C	0.3604	-1.1181	0.7709	3172.3 3174.7 3183.4 3184.4		
		H	0.4915	-2.1877	0.9635			
		H	-0.0268	-0.6647	1.6867			
		C	1.6939	-0.5000	0.4142			

		C	2.5991	-1.1022	-0.4353			
		C	2.0894	0.7587	0.9020			
		C	3.8152	-0.6059	-0.8339			
		C	3.3123	1.3223	0.5363			
		H	1.4285	1.2918	1.5792			
		C	4.1773	0.6515	-0.3275			
		H	4.4718	-1.1497	-1.5043			
		H	3.5925	2.2921	0.9318			
		H	5.1277	1.0934	-0.6072			
IS34	-538.935830	C	2.3485	0.7489	0.1178	40.0 106.1 180.0 195.4 267.1 346.4	1269.707	2
		C	2.7703	-0.0220	-0.9752	394.9 431.6 438.5 465.5 491.2 508.7	2845.228	
		C	2.3330	-1.3847	-0.9373	548.2 569.5 614.1 685.9 688.4 716.7	3552.676	
		C	1.3764	-1.8183	-0.0597	723.6 751.9 769.6 790.4 848.3 868.0		
		C	0.6780	-0.8888	0.9329	885.0 931.5 950.1 964.2 971.8 986.8		
		C	1.5284	0.3164	1.0857	989.4 989.7 1032.8 1050.7 1065.6		
		H	3.3382	0.3625	-1.8141	1109.0 1138.8 1177.3 1181.2 1186.0		
		H	2.7271	-2.0868	-1.6663	1194.2 1216.5 1226.4 1237.9 1267.6		
		H	1.0440	-2.8504	-0.0982	1287.6 1318.3 1331.8 1359.0 1378.3		
		H	0.5108	-1.4253	1.8744	1409.3 1470.4 1473.4 1512.0 1514.2		
		C	1.3351	1.7356	0.6747	1604.9 1612.1 1638.9 3002.8 3012.4		
		H	1.6676	2.5348	1.3316	3053.5 3110.5 3146.6 3148.1 3151.9		
		C	0.0647	1.9958	-0.1340	3169.5 3170.6 3179.8 3185.5		
		H	0.3229	2.1877	-1.1825			
		H	-0.4211	2.9066	0.2284			
		C	-0.9596	0.8576	-0.0747			
		C	-0.7084	-0.4402	0.4147			
		C	-2.2534	1.1479	-0.5346			
		C	-1.7453	-1.3822	0.4328			
		C	-3.2713	0.2031	-0.5254			
		H	-2.4604	2.1472	-0.9062			
		C	-3.0169	-1.0765	-0.0340			
		H	-1.5457	-2.3738	0.8276			
		H	-4.2581	0.4655	-0.8902			
		H	-3.8021	-1.8236	-0.0072			
IS35	-538.964528	C	2.9010	0.8187	0.2166	49.8 94.2 179.4 195.4 236.4 285.0	1174.258	2
		C	3.6067	-0.2724	-0.0651	377.7 390.6 439.9 451.2 463.5 492.3	3290.201	
		C	2.8361	-1.4629	-0.4709	526.1 546.6 597.4 646.7 682.0 688.7	4345.967	
		C	1.5126	-1.5219	-0.2640	721.9 749.7 797.9 800.6 820.7 839.7		
		C	0.7770	-0.4029	0.4695	864.2 889.0 944.0 955.6 964.2 974.8		
		C	1.4711	0.9360	0.2188	982.4 993.1 1019.3 1044.4 1066.6		
		H	4.6907	-0.3061	-0.0476	1112.1 1147.3 1183.0 1190.3 1201.2		
		H	3.3620	-2.2841	-0.9474	1208.2 1223.4 1255.4 1269.6 1290.2		
		H	0.9478	-2.3943	-0.5689	1308.3 1332.9 1347.4 1379.1 1387.9		
		H	0.9145	-0.6205	1.5451	1462.7 1480.2 1524.4 1588.8 1615.9		
		C	0.8028	2.0787	-0.0062	1643.9 1670.1 1686.3 2906.2 2972.1		
		H	1.3662	2.9991	-0.1276	3002.8 3149.8 3154.0 3154.5 3160.6		
		C	-0.6848	2.1663	-0.0972	3168.0 3173.1 3186.5 3191.8		
		H	-0.9598	2.7057	-1.0134			
		H	-1.0601	2.7992	0.7214			
		C	-1.4000	0.8329	-0.0574			
		C	-0.7262	-0.3645	0.2167			
		C	-2.7844	0.8064	-0.2720			
		C	-1.4681	-1.5513	0.3060			
		C	-3.5066	-0.3774	-0.1999			
		H	-3.2994	1.7365	-0.4934			
		C	-2.8421	-1.5662	0.1008			
		H	-0.9629	-2.4796	0.5502			
		H	-4.5775	-0.3741	-0.3686			
		H	-3.3913	-2.4979	0.1765			
IS36	-538.965619	C	-2.9371	0.8848	-0.1400	48.4 91.5 169.3 197.5 245.4 285.6	1151.520	2
		C	-3.5707	-0.2794	0.1127	371.1 382.9 425.7 448.5 477.9 496.8	3335.923	
		C	-2.8078	-1.4844	0.4175	529.0 556.4 596.0 667.0 677.9 698.2	4380.509	
		C	-1.4830	-1.5396	0.2127	718.6 748.5 780.6 799.9 801.8 859.6		
		C	-0.7580	-0.3934	-0.4684	878.9 944.4 953.8 970.0 974.9 980.5		
		C	-1.4774	0.9365	-0.1784	983.8 993.4 1034.5 1066.7 1068.7		

		H	-4.6524	-0.3102	0.1816	1127.4 1152.3 1184.5 1185.1 1195.1		
		H	-3.3279	-2.3316	0.8520	1201.7 1209.6 1221.6 1252.6 1275.2		
		H	-0.9196	-2.4236	0.4866	1285.4 1320.1 1342.8 1389.1 1439.0		
		H	-0.8876	-0.5614	-1.5538	1465.8 1474.5 1519.7 1590.7 1613.9		
		C	-0.7464	2.0202	0.0055	1639.5 1675.0 1718.5 2902.3 2988.2		
		C	0.7078	2.2050	0.0800	3015.3 3151.8 3156.8 3162.8 3168.6		
		H	0.9836	2.7541	0.9889	3174.3 3184.1 3187.2 3190.1		
		H	1.0614	2.8199	-0.7594			
		C	1.4277	0.8556	0.0544			
		C	0.7477	-0.3426	-0.2116			
		C	2.8103	0.8368	0.2714			
		C	1.4961	-1.5259	-0.2943			
		C	3.5343	-0.3471	0.2063			
		H	3.3225	1.7695	0.4875			
		C	2.8706	-1.5369	-0.0885			
		H	0.9961	-2.4578	-0.5338			
		H	4.6050	-0.3414	0.3765			
		H	3.4204	-2.4687	-0.1585			
		H	-3.4858	1.8139	-0.2432			
IS37	-539.543355	C	1.3329	1.5705	0.0000	-13.9 -5.0 15.6 41.6 120.8 228.2	792.863	2
		C	1.3322	2.2821	1.2023	255.7 310.2 364.1 405.2 412.1 458.7	6747.290	
		C	1.3322	3.6760	1.2046	502.9 531.5 607.5 626.6 635.9 689.2	7230.916	
		C	1.3318	4.3773	0.0000	709.5 737.8 761.2 798.0 816.6 836.8		
		C	1.3322	3.6760	-1.2046	851.0 886.8 913.4 926.2 975.8 979.3		
		C	1.3322	2.2821	-1.2023	985.6 988.8 997.5 1017.8 1033.8		
		H	1.3323	1.7417	2.1435	1045.3 1050.1 1092.3 1096.4 1158.6		
		H	1.3347	4.2134	2.1465	1177.8 1181.4 1193.6 1201.3 1211.5		
		H	1.3338	5.4615	0.0000	1279.9 1300.1 1337.1 1344.0 1356.1		
		H	1.3347	4.2134	-2.1465	1397.7 1453.7 1454.5 1481.4 1494.9		
		H	1.3323	1.7417	-2.1435	1525.4 1575.7 1601.8 1624.6 1642.1		
		C	1.3138	0.0479	0.0000	2926.2 2945.3 3154.3 3156.7 3158.9		
		H	1.8725	-0.3175	0.8779	3164.8 3167.6 3175.9 3177.3 3181.9		
		H	1.8725	-0.3175	-0.8779	3187.5 3189.7		
		C	-0.0446	-0.5144	0.0000			
		C	-0.7887	-1.7137	0.0000			
		C	-1.2014	-2.3262	-1.2148			
		C	-1.2014	-2.3262	1.2148			
		C	-1.9588	-3.4885	-1.2082			
		H	-0.9151	-1.8670	-2.1541			
		C	-1.9588	-3.4885	1.2082			
		H	-0.9151	-1.8670	2.1541			
		C	-2.3419	-4.0775	0.0000			
		H	-2.2574	-3.9397	-2.1483			
		H	-2.2574	-3.9397	2.1483			
		H	-2.9373	-4.9833	0.0000			
IS38	-539.549731	C	1.8639	0.3470	0.3601	16.4 20.1 58.1 133.6 149.9 211.9	824.218	2
		C	3.0220	1.1220	0.2558	276.3 312.7 413.3 413.7 425.0 492.4	6377.151	
		C	4.2367	0.5480	-0.1211	520.1 535.3 598.9 621.6 635.4 669.6	6497.982	
		C	4.3090	-0.8147	-0.3986	696.7 712.6 737.7 759.5 806.4 828.0		
		C	3.1591	-1.5989	-0.2981	841.5 854.7 915.5 920.0 939.5 967.2		
		C	1.9483	-1.0217	0.0750	969.2 982.7 999.1 1016.7 1022.2		
		H	2.9750	2.1842	0.4745	1049.2 1074.7 1096.9 1119.1 1163.4		
		H	5.1247	1.1663	-0.1954	1179.3 1181.9 1202.3 1212.0 1218.8		
		H	5.2519	-1.2637	-0.6899	1269.5 1306.2 1323.5 1339.1 1359.4		
		H	3.2065	-2.6614	-0.5103	1413.3 1439.4 1460.5 1469.2 1482.5		
		H	1.0574	-1.6372	0.1473	1524.4 1531.4 1578.2 1622.1 1641.1		
		C	0.5364	0.9667	0.7663	2987.5 3043.5 3151.5 3152.7 3155.9		
		H	0.7159	2.0098	1.0615	3157.4 3159.7 3167.4 3171.8 3175.3		
		H	0.1437	0.4597	1.6541	3185.6 3186.9		
		C	-0.4901	0.9239	-0.3245			
		C	-1.7955	0.4259	-0.1727			
		C	-2.3098	-0.1129	1.0213			
		C	-2.7407	0.4255	-1.2546			
		C	-3.5643	-0.6126	1.2269			
		C	-4.0226	-0.0677	-1.0940			

		H	-2.4240	0.8234	-2.2139			
		C	-4.4535	-0.5900	0.1360			
		H	-3.8742	-1.0108	2.1874			
		H	-4.7076	-0.0513	-1.9344			
		H	-5.4616	-0.9726	0.2494			
		H	-0.2010	1.3107	-1.2972			
IS39	-539.537845	C	-2.0360	-0.9889	0.3143	41.9 68.8 100.1 141.6 213.9 241.1	955.825	2
		C	-3.2645	-0.9742	-0.2630	306.4 328.8 403.7 412.9 462.7 499.5	4575.938	
		C	-3.8703	0.2881	-0.5175	523.0 553.5 577.2 625.9 655.8 682.7	5331.427	
		C	-3.1130	1.4858	-0.3892	683.7 741.0 756.4 759.6 803.4 824.9		
		C	-1.8404	1.5127	0.1159	877.3 890.2 907.1 952.0 961.3 969.7		
		C	-1.2805	0.2563	0.7115	973.0 982.7 984.0 1003.7 1023.9		
		H	-3.7395	-1.8850	-0.6158	1035.5 1057.7 1071.5 1105.1 1116.4		
		H	-4.8713	0.3349	-0.9289	1144.6 1154.7 1175.5 1192.1 1195.4		
		H	-3.5619	2.4122	-0.7342	1215.0 1263.5 1315.6 1331.6 1350.6		
		H	-1.2900	2.4446	0.1809	1366.3 1415.5 1421.9 1452.4 1466.0		
		H	-1.2639	0.3802	1.8182	1506.7 1526.6 1573.3 1598.6 1615.2		
		C	-0.7847	-1.8472	0.2802	2793.2 2962.3 3023.8 3149.3 3151.8		
		H	-0.6545	-2.4810	-0.6046	3159.1 3164.9 3173.3 3177.7 3185.3		
		H	-0.6241	-2.4731	1.1713	3188.6 3192.0		
		C	-0.0196	-0.5280	0.3253			
		C	1.3299	-0.1957	0.1228			
		C	2.2877	-1.1939	-0.2185			
		C	1.7974	1.1438	0.2510			
		C	3.6183	-0.8672	-0.4171			
		H	1.9630	-2.2231	-0.3225			
		C	3.1316	1.4548	0.0510			
		H	1.0950	1.9262	0.5124			
		C	4.0540	0.4569	-0.2858			
		H	4.3284	-1.6450	-0.6761			
		H	3.4638	2.4820	0.1562			
		H	5.0967	0.7070	-0.4423			
IS40	-539.479158	C	2.1279	0.9758	0.2727	103.6 120.3 189.5 235.0 263.4 320.5	1113.203	1
		C	3.1737	0.2592	-0.1768	366.5 394.9 445.0 502.7 513.0 532.7	3163.825	
		C	3.0271	-1.2291	-0.1183	537.1 574.2 604.0 632.4 653.8 701.0	4054.049	
		C	1.8172	-1.8518	-0.1696	708.0 764.2 779.5 811.2 845.4 853.8		
		C	0.6473	-0.8880	-0.3072	890.4 910.2 930.6 949.1 958.9 967.0		
		C	0.9348	0.1896	0.6812	972.7 978.2 983.7 1048.2 1068.9		
		H	4.0699	0.6781	-0.6246	1103.8 1110.5 1132.6 1155.2 1166.9		
		H	3.9329	-1.8276	-0.1085	1174.0 1181.2 1192.5 1207.6 1230.2		
		H	1.7460	-2.9336	-0.2055	1239.4 1254.0 1308.7 1338.6 1377.0		
		H	0.8832	-0.1101	1.7376	1385.8 1400.2 1426.5 1440.6 1449.3		
		C	1.2596	2.2743	0.2041	1537.1 1540.9 1612.8 1647.3 1667.6		
		H	1.3457	2.9021	-0.6849	2918.7 2939.6 2988.9 3025.2 3090.9		
		H	1.3693	2.9059	1.0923	3147.0 3149.0 3155.1 3156.8 3169.4		
		C	0.0358	1.3045	0.2631	3174.4 3178.5		
		C	-1.0932	0.7623	-0.2589			
		C	-2.4401	1.2221	-0.4999			
		C	-0.9172	-0.7976	-0.4069			
		C	-3.4469	0.3599	-0.1840			
		H	-2.6524	2.2579	-0.7464			
		C	-1.9584	-1.5045	0.4103			
		H	-1.1938	-1.0030	-1.4545			
		C	-3.1897	-0.9484	0.4141			
		H	-4.4769	0.6935	-0.2537			
		H	-1.7619	-2.4603	0.8845			
		H	-4.0197	-1.4552	0.8956			
		H	0.8900	-0.4182	-1.2752			
IS41	-539.478705	C	2.4937	0.9965	0.2736	72.1 93.2 129.7 186.9 225.0 241.4	1357.641	2
		C	3.4311	0.0543	0.2538	353.0 363.6 408.9 435.5 454.2 481.2	3027.233	
		C	2.9911	-1.3582	0.1823	515.5 558.1 583.3 594.1 647.0 659.6	4202.845	
		C	1.7261	-1.6688	-0.1567	687.4 703.0 736.6 761.1 762.6 810.3		
		C	0.8165	-0.5409	-0.5610	833.2 863.7 894.8 913.8 930.9 953.2		
		C	1.0488	0.6932	0.3521	964.9 965.7 973.7 993.9 1025.3		
		H	4.4914	0.2759	0.3248	1052.2 1063.0 1113.1 1129.7 1151.3		

		H	3.7191	-2.1320	0.4042	1164.3 1177.4 1188.1 1237.4 1243.7		
		H	1.4050	-2.7019	-0.2325	1271.7 1280.0 1309.4 1313.9 1337.6		
		H	0.8508	0.3898	1.3970	1343.8 1373.0 1399.0 1418.4 1435.9		
		C	-0.0406	2.9596	-0.1301	1514.7 1577.1 1581.4 1650.5 1661.6		
		H	-0.9071	3.5371	-0.4318	2850.8 2915.9 2945.7 3138.0 3149.6		
		H	0.8709	3.5030	0.0875	3153.8 3157.2 3159.9 3174.4 3178.9		
		C	-0.0889	1.6220	-0.0419	3187.6 3224.9		
		C	-1.2196	0.7222	-0.2510			
		C	-2.5474	0.9037	0.0806			
		C	-0.7315	-0.6584	-0.6604			
		C	-3.3702	-0.2133	0.2944			
		H	-2.9236	1.8951	0.3137			
		C	-1.5072	-1.7573	0.0094			
		H	-0.9677	-0.7726	-1.7374			
		C	-2.8017	-1.5241	0.3607			
		H	-4.4083	-0.0715	0.5707			
		H	-1.0763	-2.7494	0.0879			
		H	-3.4136	-2.3355	0.7408			
		H	1.1584	-0.2203	-1.5592			
IS42	-539.552631	C	-2.4514	0.9663	-0.2138	56.7 71.9 133.3 202.8 212.3 273.9	1426.661	2
		C	-3.2979	-0.1087	-0.4837	368.9 395.3 405.0 436.9 458.3 506.9	2929.786	
		C	-2.8039	-1.4542	-0.4213	535.1 552.2 580.4 591.9 594.0 672.8	4096.365	
		C	-1.5757	-1.7375	0.0829	673.4 696.2 722.7 764.6 770.1 783.3		
		C	-0.7842	-0.6469	0.7471	793.1 817.3 840.6 917.5 921.7 926.9		
		C	-1.1635	0.7320	0.2502	968.3 969.9 990.8 992.1 1013.2		
		H	-4.2934	0.0722	-0.8716	1047.5 1093.0 1095.5 1128.2 1144.0		
		H	-3.4220	-2.2521	-0.8197	1161.5 1171.2 1198.0 1226.3 1241.1		
		H	-1.2098	-2.7578	0.1128	1271.2 1274.5 1296.0 1298.9 1342.4		
		C	-0.0000	2.9531	0.0003	1386.5 1386.8 1410.3 1424.3 1426.6		
		H	0.9235	3.5138	-0.0684	1507.9 1508.6 1541.3 1595.1 1601.9		
		H	-0.9235	3.5138	-0.0684	2847.7 2872.1 3148.7 3153.4 3154.6		
		C	-0.0000	1.5915	0.1819	3156.9 3158.6 3173.3 3177.7 3187.3		
		C	1.1635	0.7320	0.2502	3188.0 3236.6		
		C	2.4514	0.9663	-0.2138			
		C	0.7842	-0.6469	0.7471			
		C	3.2979	-0.1087	-0.4837			
		H	2.7648	1.9712	-0.4791			
		C	1.5757	-1.7375	0.0829			
		H	1.0899	-0.6875	1.8110			
		C	2.8039	-1.4542	-0.4213			
		H	4.2934	0.0722	-0.8716			
		H	1.2098	-2.7578	0.1128			
		H	3.4220	-2.2521	-0.8197			
		H	-1.0899	-0.6875	1.8110			
		H	-2.7648	1.9712	-0.4791			
IS43	-539.489136	C	2.5797	0.9361	-0.3579	59.7 100.3 161.1 183.8 216.0 319.0	1146.234	1
		C	3.3379	-0.1223	0.0272	372.1 379.6 421.3 431.1 485.3 520.2	3097.399	
		C	2.7369	-1.3425	0.5640	528.8 547.3 581.1 610.8 641.1 698.4	3865.217	
		C	1.4275	-1.6183	0.3725	711.7 741.3 769.6 781.8 795.6 817.8		
		C	0.7065	-0.6551	-0.5218	856.9 887.6 926.1 957.7 967.4 968.0		
		C	1.1200	0.7986	-0.2053	976.9 979.9 994.3 1003.3 1032.5		
		H	4.4192	-0.0348	0.0300	1035.0 1065.1 1103.4 1125.4 1148.1		
		H	3.3653	-2.0119	1.1421	1168.9 1173.8 1190.0 1220.5 1238.3		
		H	0.9568	-2.4998	0.7928	1247.5 1292.1 1300.6 1315.4 1350.6		
		C	0.5508	1.8644	0.9079	1396.1 1404.4 1432.9 1453.3 1484.5		
		H	1.2559	2.6764	1.0592	1549.2 1562.7 1588.6 1636.6 1672.1		
		H	0.0414	1.5282	1.8070	2928.6 2957.3 3087.8 3147.3 3150.0		
		C	-0.0739	1.6159	-0.3912	3158.5 3163.3 3171.8 3173.1 3174.2		
		C	-1.1992	0.8521	-0.5337	3182.9 3185.9		
		C	-2.4940	1.1800	-0.0009			
		C	-0.8392	-0.6050	-0.8490			
		C	-3.3313	0.2013	0.4257			
		H	-2.7586	2.2249	0.1172			
		C	-1.7757	-1.5813	-0.1876			
		H	-0.9220	-0.8215	-1.9255			

		C	-2.9360	-1.1985	0.3715			
		H	-4.2926	0.4555	0.8582			
		H	-1.5336	-2.6362	-0.2756			
		H	-3.6132	-1.9422	0.7782			
		H	1.1889	-0.7815	-1.5039			
		H	3.0325	1.8906	-0.6078			
IS44	-539.499607	C	-2.4015	0.7812	-0.8405	65.3 76.1 160.0 192.2 260.9 280.7	1330.274	2
		C	-3.1207	-0.4394	-0.8002	328.0 367.6 412.0 450.2 467.7 493.0	3041.911	
		C	-2.7318	-1.4519	0.1106	500.6 550.4 580.5 625.9 644.9 681.4	3880.119	
		C	-1.6502	-1.2953	0.9270	697.8 727.8 742.8 779.0 786.7 807.9		
		C	-0.8002	-0.0577	0.9035	872.0 891.9 934.8 951.6 970.0 972.7		
		C	-1.3179	0.9978	-0.0402	974.3 982.7 1004.7 1016.9 1027.5		
		H	-3.9697	-0.5908	-1.4553	1051.8 1090.2 1126.6 1138.4 1150.5		
		H	-3.3111	-2.3684	0.1604	1174.6 1180.9 1193.7 1210.0 1234.9		
		H	-1.3764	-2.0783	1.6274	1243.4 1278.5 1301.3 1320.7 1348.1		
		C	-0.5615	2.3128	0.0066	1385.2 1412.0 1431.6 1433.0 1456.8		
		H	-0.8811	2.9045	0.8797	1538.9 1576.8 1603.4 1662.8 1702.4		
		H	-0.7935	2.9187	-0.8760	2883.1 2927.2 2954.2 3037.7 3145.9		
		C	0.8863	2.0237	0.0819	3148.5 3154.9 3165.9 3166.6 3177.7		
		C	1.5272	0.8830	0.2695	3186.0 3192.3		
		C	2.9495	0.6401	0.0207			
		C	0.7315	-0.3651	0.6830			
		C	3.3389	-0.5780	-0.4162			
		H	3.6459	1.4684	0.0847			
		C	1.0894	-1.5083	-0.2374			
		H	1.1224	-0.6457	1.6763			
		C	2.3525	-1.6201	-0.6835			
		H	4.3778	-0.7605	-0.6683			
		H	0.3408	-2.2610	-0.4586			
		H	2.6521	-2.4771	-1.2777			
		H	-0.8251	0.3885	1.9155			
		H	-2.7304	1.5645	-1.5176			
Phenanthrene	-538.516476	C	3.5570	-0.2966	0.0000	95.0 100.1 226.9 241.9 247.1 401.1	1115.111	1
		C	2.8347	0.8775	0.0000	411.2 436.9 446.1 506.0 507.5 543.7	3272.744	
		C	1.4214	0.8651	0.0000	556.9 599.3 631.8 722.8 725.5 726.7	4387.855	
		C	0.7284	-0.3795	0.0000	747.0 766.9 798.7 827.2 842.9 872.0		
		C	1.4982	-1.5648	-0.0000	879.6 887.7 956.4 966.3 981.3 991.5		
		C	2.8787	-1.5279	-0.0000	991.6 1016.5 1060.2 1060.5 1114.4		
		C	0.6786	2.0920	0.0000	1165.0 1173.3 1185.8 1188.9 1224.1		
		C	-0.7284	-0.3795	0.0000	1241.8 1265.6 1304.1 1324.0 1367.8		
		C	-1.4214	0.8651	-0.0000	1374.3 1444.4 1449.4 1469.6 1489.1		
		C	-0.6786	2.0920	-0.0000	1533.5 1560.3 1606.1 1640.4 1652.8		
		C	-2.8347	0.8775	-0.0000	1657.7 3155.3 3158.5 3159.3 3168.1		
		H	-3.3460	1.8346	-0.0000	3169.5 3175.3 3182.0 3185.1 3192.0		
		C	-3.5570	-0.2966	0.0000	3204.3		
		C	-2.8787	-1.5279	0.0000			
		C	-1.4982	-1.5648	0.0000			
		H	1.2289	3.0271	0.0000			
		H	4.6408	-0.2728	0.0000			
		H	3.3460	1.8346	0.0000			
		H	1.0062	-2.5287	-0.0000			
		H	3.4411	-2.4548	-0.0000			
		H	-1.2289	3.0271	-0.0000			
		H	-4.6408	-0.2728	-0.0000			
		H	-3.4411	-2.4548	0.0000			
		H	-1.0062	-2.5287	0.0000			
H	-0.499818	H	0.0000	0.0000	0.0000	0	0	2
H2	-1.166086	H	2.8561	-0.6965	0.1412	4418.0	0.000	1
		H	3.6002	-0.6921	0.1412		0.996	
							0.996	
Benzyl	-270.378161	C	-2.6142	-0.6770	0.3710	198.4 358.6 389.5 478.4 503.2 533.9	325.476	2
		C	-1.8782	-1.8448	0.1331	627.5 682.2 712.6 780.9 830.1 830.3	667.189	
		C	-0.4930	-1.7618	-0.0582	900.1 969.0 971.8 984.4 994.2	992.664	
		C	0.1497	-0.5373	-0.0136	1034.5 1115.6 1174.5 1184.6 1286.8		

		C	-0.5747	0.6668	0.2268	1327.8 1351.8 1471.2 1488.7 1500.3		
		C	-1.9830	0.5533	0.4180	1574.1 1594.8 3144.0 3157.6 3160.3		
		H	-3.6869	-0.7372	0.5196	3172.3 3177.0 3189.9 3240.8		
		H	-2.3771	-2.8062	0.0972			
		H	0.0803	-2.6638	-0.2427			
		H	-2.5594	1.4537	0.6027			
		H	1.2228	-0.4806	-0.1626			
		C	0.0720	1.9130	0.2733			
		H	1.1419	1.9937	0.1274			
		H	-0.4829	2.8247	0.4562			
TS2	-541.337318	C	1.8902	-0.0582	-0.3627	-866.7 20.3 36.2 53.7 60.9 117.1	765.576	2
		C	2.6264	-1.2531	-0.2980	172.7 231.4 248.9 288.8 318.1 369.8	6793.678	
		C	3.9902	-1.2477	-0.0051	413.3 417.1 483.0 528.5 538.0 618.6	7379.573	
		C	4.6606	-0.0484	0.2315	622.6 636.1 705.0 711.8 748.5 764.6		
		C	3.9554	1.1590	0.1716	769.9 801.4 850.9 854.1 867.3 913.7		
		C	2.6089	1.1015	-0.1189	923.1 946.8 964.7 980.7 985.9 996.7		
		H	2.1199	-2.1953	-0.4870	997.2 1010.5 1017.2 1027.3 1049.7		
		H	4.5326	-2.1857	0.0338	1055.2 1093.0 1126.1 1167.1 1177.4		
		H	5.7218	-0.0471	0.4560	1181.3 1202.1 1216.4 1223.0 1273.3		
		H	4.4556	2.1061	0.3447	1296.2 1311.3 1331.0 1341.3 1360.9		
		H	1.9020	2.4168	-0.2074	1362.2 1452.3 1479.9 1482.3 1487.4		
		C	0.4043	-0.0558	-0.6429	1504.0 1525.7 1580.2 1622.2 1629.8		
		H	0.1388	-0.9511	-1.2128	1643.2 2332.5 3028.8 3040.3 3062.0		
		H	0.1464	0.8038	-1.2677	3085.8 3146.5 3150.4 3152.5 3159.0		
		C	-0.4479	-0.0095	0.6506	3165.5 3170.9 3174.2 3184.0 3186.7		
		H	-0.1780	0.8865	1.2175			
		H	-0.1865	-0.8679	1.2772			
		C	-1.9333	-0.0125	0.3681			
		C	-2.6221	1.1845	0.1401			
		C	-2.6487	-1.2129	0.2939			
		C	-3.9840	1.1833	-0.1555			
		H	-2.0872	2.1274	0.2010			
		C	-4.0109	-1.2199	-0.0015			
		H	-2.1350	-2.1520	0.4764			
		C	-4.6835	-0.0204	-0.2285			
		H	-4.4998	2.1223	-0.3240			
		H	-4.5475	-2.1612	-0.0493			
		H	-5.7437	-0.0231	-0.4551			
		H	1.5267	3.1803	-0.2589			
TS3	-540.174655	C	1.4198	-0.7945	-0.0739	-327.7 47.7 78.7 132.2 187.7 212.8	1376.049	2
		C	2.7930	-0.8188	-0.3759	238.7 356.4 391.8 412.0 416.1 482.3	3397.013	
		C	3.5448	0.3543	-0.4126	510.1 529.2 591.9 601.8 625.6 696.8	4307.370	
		C	2.9463	1.5861	-0.1460	716.8 741.4 749.7 764.6 780.1 846.9		
		C	1.5843	1.6357	0.1696	859.5 880.2 906.6 942.0 944.8 966.7		
		C	0.8762	0.4520	0.1947	982.1 983.9 998.0 1019.2 1023.2		
		H	3.2726	-1.7707	-0.5885	1043.0 1048.1 1087.7 1123.2 1173.9		
		H	4.6019	0.3062	-0.6491	1176.6 1177.5 1187.6 1196.4 1217.6		
		H	3.5325	2.4988	-0.1769	1221.4 1276.9 1320.5 1331.5 1337.6		
		H	1.1032	2.5844	0.3879	1355.2 1375.7 1447.5 1462.2 1472.4		
		C	0.6005	-2.0721	-0.1064	1484.9 1494.7 1517.1 1577.2 1586.7		
		H	1.2247	-2.9122	0.2151	1607.6 1626.7 3007.1 3025.5 3050.1		
		H	0.3203	-2.2784	-1.1469	3069.5 3138.9 3146.2 3150.2 3153.2		
		C	-0.6897	-2.0345	0.7455	3162.1 3163.3 3176.1 3180.0 3186.6		
		H	-0.4202	-2.0097	1.8064			
		H	-1.2504	-2.9581	0.5748			
		C	-1.5281	-0.8325	0.4004			
		C	-1.1944	0.4130	1.0029			
		C	-2.4792	-0.8568	-0.6112			
		C	-1.9053	1.5791	0.6311			
		H	-0.6721	0.4072	1.9529			
		C	-3.1342	0.3127	-1.0153			
		H	-2.7164	-1.7985	-1.0972			
		C	-2.8409	1.5295	-0.3919			
		H	-1.7094	2.5124	1.1471			
		H	-3.8783	0.2709	-1.8025			

		H	-3.3679	2.4296	-0.6890			
TS4	-540.181956	C	-1.4178	0.8095	-0.1956	-905.1 88.7 98.9 172.6 207.7 263.7		2
		C	-2.8111	0.8241	-0.2997	312.2 380.5 395.7 421.0 441.1 470.2		
		C	-3.5604	-0.3345	-0.1183	491.5 511.4 530.7 553.5 578.3 608.4		
		C	-2.9124	-1.5306	0.1868	636.3 712.1 736.3 749.2 758.3 782.5		
		C	-1.5268	-1.5577	0.2945	798.2 816.6 876.4 879.7 907.9 955.3		
		C	-0.7607	-0.4026	0.0895	960.2 985.9 990.4 992.3 1020.5		
		H	-3.3132	1.7608	-0.5206	1047.7 1063.4 1069.1 1109.3 1149.5		
		H	-4.6411	-0.3018	-0.1991	1180.5 1182.9 1186.7 1203.6 1216.3		
		H	-3.4850	-2.4362	0.3527	1223.3 1273.1 1288.9 1304.2 1324.0		
		H	-1.0357	-2.4859	0.5627	1334.1 1358.7 1381.3 1469.0 1470.3		
		C	-0.6108	2.0745	-0.3902	1480.7 1483.0 1504.7 1520.0 1582.1		
		H	-1.2265	2.9471	-0.1556	1615.3 1625.5 1643.2 2986.8 3001.1		
		H	-0.3211	2.1672	-1.4455	3062.5 3069.9 3153.7 3155.8 3165.4		
		C	0.6514	2.0581	0.4808	3167.9 3177.1 3183.9 3188.3 3194.8		
		H	0.3551	2.0865	1.5389			
		H	1.2662	2.9422	0.2946			
		C	1.4442	0.8052	0.2227			
		C	0.7343	-0.4328	0.1564			
		C	2.8270	0.8106	0.0950			
		C	1.4605	-1.5931	-0.2256			
		H	0.7725	-0.7091	1.9253			
		C	3.5341	-0.3654	-0.1636			
		H	3.3620	1.7509	0.1846			
		C	2.8399	-1.5640	-0.3450			
		H	0.9281	-2.5196	-0.4008			
		H	4.6134	-0.3394	-0.2611			
		H	3.3773	-2.4699	-0.6019			
TS5	-540.185239	C	-1.4384	0.7700	-0.2315	-849.8 87.3 98.2 164.0 188.4 241.0	1227.339	2
		C	-2.8338	0.7752	-0.2219	276.4 297.9 353.3 394.1 410.5 463.4	3340.427	
		C	-3.5557	-0.3919	0.0116	466.9 492.0 517.3 556.0 576.4 632.9	4428.197	
		C	-2.8739	-1.5836	0.2523	641.1 721.0 737.6 745.6 760.3 793.1		
		C	-1.4839	-1.6010	0.2460	802.6 821.7 879.7 880.5 913.3 959.3		
		C	-0.7425	-0.4367	-0.0090	960.1 989.2 991.8 1004.7 1022.5		
		H	-3.3597	1.7091	-0.3935	1050.4 1068.4 1071.2 1113.2 1152.0		
		H	-4.6396	-0.3689	0.0205	1170.5 1184.0 1188.8 1208.1 1223.0		
		H	-3.4234	-2.4958	0.4560	1227.1 1274.1 1303.3 1305.2 1311.1		
		H	-0.9704	-2.5299	0.4619	1329.7 1345.8 1363.0 1386.6 1455.1		
		C	-0.6576	2.0365	-0.4938	1468.5 1483.7 1489.6 1519.7 1522.9		
		H	-1.2582	2.9114	-0.2307	1598.4 1620.1 1636.2 1645.4 2976.8		
		H	-0.4432	2.1156	-1.5701	3062.5 3080.2 3155.1 3156.8 3166.2		
		C	0.6604	2.0440	0.2657	3168.4 3178.6 3183.3 3189.2 3194.7		
		H	0.3781	2.1765	1.4327			
		H	1.2624	2.9308	0.0573			
		C	1.4351	0.7845	0.1122			
		C	0.7398	-0.4381	-0.0373			
		C	2.8341	0.7873	0.1341			
		C	1.4850	-1.6139	-0.2063			
		C	3.5566	-0.3916	-0.0128			
		H	3.3570	1.7301	0.2593			
		C	2.8757	-1.5958	-0.1922			
		H	0.9751	-2.5560	-0.3666			
		H	4.6404	-0.3714	-0.0013			
		H	3.4274	-2.5193	-0.3277			
		H	0.0489	2.3985	2.4996			
TS5’	-539.735276	C	-1.4309	0.8792	0.0510	-1608.1 46.4 87.1 177.8 189.5 245.6	1199.532	3
		C	-2.8838	0.8558	0.0469	264.7 354.0 387.9 423.6 434.1 452.5	3328.681	
		C	-3.5697	-0.3134	0.0114	472.9 518.3 537.0 548.4 594.6 617.3	4493.160	
		C	-2.8639	-1.5631	-0.0285	687.9 694.4 704.9 718.4 747.5 771.4		
		C	-1.4773	-1.5859	-0.0442	813.8 818.3 850.4 856.5 916.5 930.7		
		C	-0.7100	-0.4151	-0.0123	962.2 976.5 984.0 993.1 1009.0		
		H	-3.4061	1.8061	0.0720	1019.9 1031.9 1065.0 1099.7 1138.3		
		H	-4.6539	-0.3139	0.0112	1163.9 1188.4 1197.0 1207.2 1213.7		
		H	-3.4197	-2.4925	-0.0517	1245.0 1291.5 1300.7 1331.9 1371.2		
		H	-0.9858	-2.5498	-0.0757	1383.2 1410.1 1434.5 1443.4 1485.1		
		C	-0.7490	2.0735	-0.0402	1490.8 1512.5 1566.3 1586.7 1618.4		

		H	-1.3071	2.9893	0.1374	1633.0 2947.0 2962.1 3130.0 3152.1		
		H	-0.8107	2.3999	-1.6651	3161.5 3168.1 3175.8 3182.6 3186.8		
		C	0.7392	2.1526	0.1331	3194.8 3205.9		
		H	0.9558	2.6553	1.0887			
		H	1.1675	2.8163	-0.6347			
		C	1.4485	0.8249	0.0947			
		C	0.7399	-0.4049	0.0060			
		C	2.8471	0.8166	0.1303			
		C	1.5024	-1.6000	-0.0475			
		C	3.5694	-0.3661	0.0837			
		H	3.3734	1.7645	0.1917			
		C	2.8818	-1.5847	-0.0081			
		H	0.9988	-2.5545	-0.1238			
		H	4.6527	-0.3478	0.1121			
		H	3.4321	-2.5179	-0.0515			
TS6	-539.010128	C	-1.4272	0.8478	-0.0515	-628.7 92.9 99.5 202.8 232.7 248.9	1152.670	2
		C	-2.8418	0.8659	-0.0704	297.7 347.5 408.8 423.2 437.8 446.6	3292.446	
		C	-3.5690	-0.3038	-0.0215	507.1 513.1 548.8 558.0 600.7 631.7	4416.353	
		C	-2.8959	-1.5357	0.0494	722.2 725.7 730.6 751.5 767.4 798.0		
		C	-1.5145	-1.5786	0.0641	840.5 842.7 874.1 880.9 887.8 958.3		
		C	-0.7395	-0.4002	0.0105	966.5 987.6 992.6 998.5 1016.6		
		H	-3.3483	1.8241	-0.1202	1060.3 1061.7 1113.3 1164.5 1168.1		
		H	-4.6526	-0.2760	-0.0338	1182.4 1188.9 1222.6 1237.8 1264.0		
		H	-3.4623	-2.4591	0.0929	1304.8 1320.9 1364.4 1371.5 1441.3		
		H	-1.0279	-2.5436	0.1206	1448.0 1463.4 1488.8 1528.8 1556.2		
		C	-0.6843	2.0663	-0.0950	1604.8 1618.4 1643.3 1650.9 3159.6		
		H	-1.2274	3.0035	-0.1521	3160.4 3164.2 3169.5 3170.8 3180.4		
		C	0.6845	2.0681	-0.0168	3183.3 3186.3 3193.0 3205.4		
		H	0.8820	2.5389	1.8992			
		H	1.2362	2.9919	-0.1467			
		C	1.4218	0.8268	-0.0206			
		C	0.7194	-0.4089	0.0030			
		C	2.8318	0.8310	-0.0434			
		C	1.4790	-1.6002	0.0022			
		C	3.5465	-0.3489	-0.0448			
		H	3.3499	1.7843	-0.0552			
		C	2.8600	-1.5741	-0.0207			
		H	0.9795	-2.5601	0.0147			
		H	4.6302	-0.3324	-0.0636			
		H	3.4152	-2.5053	-0.0219			
TS7	-539.544338	C	-1.4388	0.7945	-0.1805	-674.9 81.5 91.7 166.1 191.8 251.6	1203.379	1
		C	-2.8339	0.8096	-0.1101	277.8 382.0 396.9 421.5 432.2 461.4	3316.586	
		C	-3.5516	-0.3640	0.0893	471.1 510.1 529.8 557.3 567.8 631.4	4419.591	
		C	-2.8691	-1.5743	0.2292	676.3 717.5 731.0 744.9 775.7 792.4		
		C	-1.4828	-1.6009	0.1659	819.4 825.5 872.2 883.8 898.3 955.3		
		C	-0.7435	-0.4239	-0.0482	962.8 984.8 992.8 1005.3 1021.4		
		H	-3.3583	1.7550	-0.2095	1048.1 1065.8 1074.3 1112.2 1138.0		
		H	-4.6341	-0.3380	0.1449	1154.0 1185.1 1187.5 1201.9 1211.7		
		H	-3.4186	-2.4931	0.4000	1251.6 1270.2 1294.0 1312.6 1323.4		
		H	-0.9710	-2.5447	0.3078	1336.1 1363.7 1397.8 1458.5 1477.8		
		C	-0.6533	2.0577	-0.4157	1498.9 1515.2 1582.5 1615.5 1630.2		
		H	-1.2163	2.9421	-0.1056	1641.7 2928.9 3003.5 3066.7 3154.2		
		H	-0.5174	2.1807	-1.5078	3162.7 3167.8 3175.3 3180.3 3186.1		
		C	0.7670	2.1189	0.0387	3191.3 3196.6		
		H	0.3757	2.4175	2.0098			
		H	0.7865	2.7441	1.3691			
		C	1.4291	0.8191	0.0752			
		C	0.7309	-0.4128	-0.0867			
		C	2.8350	0.8056	0.1782			
		C	1.4824	-1.5906	-0.2302			
		C	3.5556	-0.3722	0.0775			
		H	3.3357	1.7583	0.3092			
		C	2.8687	-1.5706	-0.1476			
		H	0.9849	-2.5354	-0.4112			
		H	4.6372	-0.3660	0.1456			
		H	3.4220	-2.4967	-0.2618			
TS8	-538.388946	C	-1.4301	0.8826	0.0190	-895.1 80.8 87.5 214.3 230.4 247.4	1122.839	1

		C	-2.8392	0.8891	0.0150	398.4 407.7 434.1 446.2 488.2 503.4	3278.611	
		C	-3.5695	-0.2865	-0.0052	545.8 552.8 598.4 631.3 696.7 719.3	4392.649	
		C	-2.8907	-1.5105	-0.0158	728.3 756.7 777.8 805.2 821.8 833.2		
		C	-1.5049	-1.5502	-0.0093	878.1 890.1 898.7 966.5 983.0 996.0		
		C	-0.7430	-0.3668	0.0070	1008.4 1021.0 1063.3 1065.1 1110.5		
		H	-3.3279	1.8561	0.0326	1150.4 1166.7 1186.7 1188.6 1221.8		
		H	-4.6533	-0.2631	-0.0103	1251.2 1258.4 1283.0 1302.3 1338.8		
		H	-3.4502	-2.4398	-0.0282	1346.2 1351.9 1414.3 1455.3 1479.2		
		H	-1.0171	-2.5165	-0.0175	1508.2 1519.5 1583.1 1613.6 1635.4		
		C	-0.7638	2.1852	0.1124	1646.3 2216.4 3088.5 3158.1 3162.9		
		C	0.6510	2.0970	0.0066	3169.8 3177.5 3184.9 3189.3 3194.3		
		H	1.2308	3.0088	0.1602	3204.8		
		H	0.0570	2.4081	-1.0225			
		C	1.4244	0.8433	-0.0014			
		C	0.7269	-0.3851	0.0025			
		C	2.8261	0.8647	-0.0010			
		C	1.4854	-1.5726	0.0044			
		C	3.5516	-0.3151	0.0042			
		H	3.3374	1.8222	0.0004			
		C	2.8705	-1.5384	0.0051			
		H	0.9914	-2.5352	0.0076			
		H	4.6353	-0.2933	0.0090			
		H	3.4289	-2.4678	0.0082			
TS9	-539.531927	C	1.4290	0.8381	0.1287	-2184.7 86.0 96.9 194.1 215.2 259.1	1184.854	1
		C	2.8357	0.8259	0.2587	314.8 391.2 420.4 448.9 449.7 491.3	3309.924	
		C	3.5598	-0.3452	0.1239	516.0 548.2 574.9 591.8 631.9 649.3	4429.945	
		C	2.9047	-1.5511	-0.1576	715.4 729.4 732.6 746.2 763.0 784.0		
		C	1.5211	-1.5669	-0.2568	819.2 834.8 862.7 879.8 913.2 949.7		
		C	0.7564	-0.4004	-0.0932	961.8 979.8 993.2 1017.0 1061.9		
		H	3.3492	1.7617	0.4537	1066.7 1076.6 1096.5 1126.6 1150.5		
		H	4.6401	-0.3238	0.2191	1159.7 1186.3 1194.5 1206.8 1245.4		
		H	3.4708	-2.4649	-0.2933	1257.2 1297.0 1304.4 1333.5 1340.0		
		H	1.0262	-2.5071	-0.4681	1348.6 1372.9 1421.1 1473.8 1486.6		
		C	0.6838	2.0619	0.2208	1518.1 1524.1 1583.0 1611.3 1636.6		
		H	0.1334	2.2782	-1.1002	1645.8 2064.8 3154.4 3158.7 3165.7		
		H	1.1565	2.9929	0.5011	3167.6 3169.5 3176.3 3187.9 3190.8		
		C	-0.7258	2.0720	-0.1857	3201.1 3201.7		
		H	-0.8702	2.3404	-1.6958			
		H	-1.2820	2.9678	0.0629			
		C	-1.4494	0.7849	-0.0759			
		C	-0.7172	-0.4222	-0.0488			
		C	-2.8440	0.7860	0.0075			
		C	-1.4532	-1.6144	0.0829			
		C	-3.5472	-0.4050	0.1257			
		H	-3.3768	1.7309	-0.0290			
		C	-2.8391	-1.6083	0.1621			
		H	-0.9335	-2.5617	0.1440			
		H	-4.6289	-0.3997	0.1895			
		H	-3.3720	-2.5473	0.2629			
TS10	-541.353063	C	-1.9153	-0.0971	0.2110	-951.6 19.8 36.6 50.3 64.8 138.5	746.184	2
		C	-2.7326	-1.1753	0.5836	201.0 242.4 294.4 326.8 344.2 407.0	6947.002	
		C	-4.1126	-1.1285	0.4060	412.6 413.6 499.3 529.6 538.9 628.0	7303.839	
		C	-4.7089	0.0037	-0.1472	634.9 636.2 706.1 711.4 755.1 765.4		
		C	-3.9118	1.0863	-0.5177	807.6 819.4 849.9 854.3 862.2 920.0		
		C	-2.5317	1.0374	-0.3392	927.2 980.7 982.1 998.2 999.0		
		H	-2.2768	-2.0614	1.0138	1015.0 1017.2 1018.2 1034.7 1050.0		
		H	-4.7220	-1.9768	0.6976	1051.1 1097.7 1110.9 1171.2 1181.7		
		H	-5.7831	0.0429	-0.2875	1182.1 1202.9 1205.1 1219.4 1224.7		
		H	-4.3665	1.9727	-0.9460	1272.8 1281.5 1332.3 1339.6 1345.3		
		H	-1.9320	1.8926	-0.6289	1352.5 1360.6 1383.5 1404.3 1481.8		
		C	-0.4425	-0.1666	0.4435	1482.7 1488.1 1525.2 1526.7 1615.8		
		H	-0.1293	-1.1835	0.6912	1622.8 1639.1 1643.8 3017.9 3061.3		
		H	-0.2067	0.4324	1.4792	3077.6 3150.4 3155.4 3156.9 3162.4		
		C	0.4784	0.4527	-0.6168	3167.0 3172.1 3175.7 3180.2 3187.4		
		H	0.2941	1.5282	-0.6882	3189.1		

		H	0.2136	0.0275	-1.5921		
		C	1.9469	0.2109	-0.3416		
		C	2.7187	1.1541	0.3450		
		C	2.5608	-0.9786	-0.7511		
		C	4.0646	0.9154	0.6190		
		H	2.2625	2.0842	0.6681		
		C	3.9057	-1.2216	-0.4801		
		H	1.9814	-1.7190	-1.2946		
		C	4.6625	-0.2743	0.2081		
		H	4.6459	1.6603	1.1513		
		H	4.3637	-2.1475	-0.8105		
		H	5.7099	-0.4599	0.4177		
		H	0.0512	0.9962	2.3935		
TS10’	-540.915912	C	-0.1763	1.6553	-0.0190	-1661.3 15.8 29.1 51.3 105.1 169.0	1045.439
		C	-1.5993	1.6895	0.3405	187.2 255.7 321.4 332.2 399.0 412.4	5606.950
		C	-2.4530	2.5633	-0.2620	436.5 478.8 507.6 544.2 571.1 588.8	5880.695
		C	-1.9920	3.4884	-1.2468	629.7 634.9 636.1 710.7 741.3 753.1	
		C	-0.6082	3.5317	-1.5713	753.8 775.6 820.2 828.1 852.6 920.1	
		C	0.2723	2.6724	-0.9844	932.5 966.2 968.6 971.5 981.7 981.9	
		H	-1.9718	1.0057	1.0923	999.0 1016.4 1032.4 1041.9 1050.0	
		H	-3.5024	2.5653	0.0122	1072.5 1096.5 1120.7 1181.1 1194.3	
		H	-2.6873	4.1684	-1.7223	1203.3 1209.0 1210.3 1254.8 1308.1	
		H	-0.2537	4.2616	-2.2908	1330.4 1342.9 1359.9 1364.8 1391.8	
		H	1.3281	2.7095	-1.2286	1445.1 1480.0 1490.2 1524.3 1535.1	
		C	0.7694	0.8821	0.6341	1544.9 1621.3 1630.3 1638.9 3036.2	
		H	1.2457	1.9088	1.7770	3077.7 3108.2 3154.4 3158.7 3163.0	
		H	1.7682	0.8912	0.1994	3166.2 3168.4 3176.4 3181.1 3187.5	
		C	0.4825	-0.3333	1.4938	3193.0 3199.8	
		H	-0.5180	-0.2718	1.9283		
		H	1.1811	-0.3465	2.3356		
		C	0.6313	-1.6309	0.7139		
		C	-0.2722	-1.9690	-0.3012		
		C	1.6801	-2.5120	0.9933		
		C	-0.1358	-3.1602	-1.0090		
		H	-1.0860	-1.2930	-0.5421		
		C	1.8230	-3.7043	0.2829		
		H	2.3894	-2.2660	1.7772		
		C	0.9145	-4.0325	-0.7201		
		H	-0.8481	-3.4077	-1.7883		
		H	2.6426	-4.3751	0.5159		
		H	1.0222	-4.9588	-1.2731		
TS11	-540.119045	C	1.9733	-0.3802	-0.2238	-2199.7 21.5 32.9 58.9 106.4 132.5	748.219
		C	2.9714	-1.2994	0.0797	232.5 290.1 336.5 388.3 412.7 426.7	6597.429
		C	4.2731	-0.7959	0.2015	478.4 517.4 545.2 628.9 632.9 636.4	7138.863
		C	4.5513	0.5650	0.0281	707.9 711.7 747.0 758.5 789.5 812.0	
		C	3.5385	1.4894	-0.2738	853.9 864.7 879.0 928.3 946.0 960.5	
		C	2.2635	0.9590	-0.3877	980.8 990.0 994.9 998.0 1017.4	
		H	2.7731	-2.3572	0.2166	1022.1 1039.1 1049.9 1100.6 1120.8	
		H	5.0878	-1.4729	0.4344	1146.0 1174.2 1180.9 1191.2 1202.2	
		H	5.5745	0.9128	0.1290	1208.2 1221.0 1268.0 1276.9 1325.4	
		H	3.7607	2.5417	-0.4051	1338.2 1358.0 1368.7 1455.1 1474.1	
		H	0.8350	1.0400	-0.6240	1479.2 1482.1 1526.3 1586.2 1623.1	
		C	0.4878	-0.3291	-0.4557	1633.6 1643.6 1792.0 2984.3 3043.2	
		H	0.1409	-0.6646	-1.4349	3085.2 3151.6 3153.1 3155.4 3163.5	
		C	-0.4687	-0.5843	0.6945	3166.7 3175.4 3178.6 3186.2 3187.3	
		H	-0.1312	-0.0199	1.5703		
		H	-0.3975	-1.6455	0.9738		
		C	-1.9075	-0.2447	0.3712		
		C	-2.3803	1.0644	0.5144		
		C	-2.7871	-1.2220	-0.1050		
		C	-3.6960	1.3886	0.1902		
		H	-1.7123	1.8354	0.8852		
		C	-4.1042	-0.9021	-0.4323		
		H	-2.4400	-2.2448	-0.2159		
		C	-4.5627	0.4055	-0.2859		
		H	-4.0454	2.4081	0.3117		
		H	-4.7720	-1.6749	-0.7970		
		H	-5.5874	0.6561	-0.5365		

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TS12	-540.159318	C	-1.9363	0.1963	-0.0016	-434.0 24.2 57.6 72.2 92.5 180.7	688.662	2
		C	-2.5020	-1.0778	-0.1984	199.5 260.9 278.5 309.7 319.3 410.5	6907.466	
		C	-3.8780	-1.2613	-0.1552	411.9 465.8 491.5 535.8 551.2 632.2	7504.553	
		C	-4.7302	-0.1802	0.0815	635.8 653.9 698.1 702.0 752.4 777.4		
		C	-4.1893	1.0901	0.2699	832.7 843.7 846.3 873.2 879.9 923.3		
		C	-2.8110	1.2745	0.2250	928.9 979.9 980.5 984.3 996.4		
		H	-1.8626	-1.9287	-0.4003	1000.1 1013.2 1014.6 1048.0 1049.8		
		H	-4.2915	-2.2512	-0.3129	1102.3 1105.1 1182.2 1182.5 1203.4		
		H	-5.8036	-0.3281	0.1126	1204.6 1209.8 1245.3 1289.2 1324.3		
		H	-4.8407	1.9380	0.4496	1339.3 1354.2 1359.9 1369.1 1473.9		
		H	-2.3971	2.2669	0.3721	1482.7 1521.2 1528.7 1605.4 1614.9		
		C	-0.4989	0.4508	-0.0255	1629.7 1640.6 1649.3 3141.1 3151.4		
		H	-0.2244	1.5012	0.0185	3157.2 3157.5 3163.5 3164.8 3173.3		
		C	0.4922	-0.4722	-0.0908	3174.4 3181.7 3184.1 3190.1 3191.2		
		H	0.3560	-0.9326	-2.1932			
		H	0.2312	-1.5241	-0.0245			
		C	1.9359	-0.1964	-0.0424			
		C	2.4854	1.0738	-0.2857			
		C	2.8162	-1.2468	0.2626			
		C	3.8567	1.2847	-0.2060			
		H	1.8389	1.9004	-0.5565			
		C	4.1898	-1.0364	0.3438			
		H	2.4138	-2.2385	0.4425			
		C	4.7171	0.2322	0.1124			
		H	4.2592	2.2726	-0.4009			
		H	4.8478	-1.8637	0.5855			
		H	5.7866	0.3996	0.1705			
TS13	-540.137824	C	-1.9661	-0.2059	0.0000	-856.2 13.8 57.2 78.3 79.1 168.5	707.744	2
		C	-2.8605	-1.2899	-0.0000	203.1 220.7 243.3 284.8 303.5 411.2	6928.248	
		C	-4.2384	-1.0922	-0.0000	414.0 467.7 482.0 545.3 546.0 620.2	7635.992	
		C	-4.7580	0.2001	0.0000	634.2 647.5 690.8 703.7 748.1 777.8		
		C	-3.8844	1.2900	0.0000	832.0 844.7 850.8 878.1 881.8 908.9		
		C	-2.5097	1.0920	0.0000	928.2 945.0 965.9 978.7 978.9 991.0		
		H	-2.4643	-2.3003	-0.0000	1002.2 1013.7 1026.9 1049.1 1057.5		
		H	-4.9051	-1.9473	-0.0000	1103.8 1122.4 1176.6 1182.5 1204.6		
		H	-5.8302	0.3596	0.0000	1207.8 1239.7 1283.4 1306.0 1327.7		
		H	-4.2796	2.2999	0.0000	1349.1 1355.7 1367.1 1447.6 1477.8		
		H	-1.8544	1.9549	0.0000	1483.1 1526.4 1574.4 1612.6 1623.4		
		C	-0.5267	-0.4820	0.0000	1638.6 1681.2 2365.3 3138.7 3156.2		
		H	-0.2774	-1.5399	0.0000	3158.7 3161.0 3165.2 3166.5 3173.8		
		C	0.4717	0.4197	0.0000	3175.6 3183.6 3186.8 3190.8		
		H	0.2289	1.4773	0.0000			
		C	1.9088	0.1327	0.0000			
		C	2.8382	1.1700	0.0000			
		C	2.4632	-1.1670	0.0000			
		C	4.2075	1.0209	0.0000			
		H	2.3456	2.5886	-0.0000			
		C	3.8391	-1.3636	0.0000			
		H	1.8074	-2.0304	0.0000			
		C	4.7209	-0.2797	0.0000			
		H	4.8673	1.8820	-0.0000			
		H	4.2311	-2.3745	0.0000			
		H	5.7929	-0.4431	0.0000			
		H	2.1035	3.4028	-0.0000			
TS14	-538.974952	C	-1.5111	0.9094	0.1879	-282.3 58.9 89.0 137.0 201.2 232.3	1248.908	2
		C	-0.6402	2.0834	0.2684	279.1 390.2 402.8 429.1 472.8 503.0	3585.351	
		C	-1.9699	-1.4275	0.7641	522.2 575.3 588.8 621.7 686.0 703.0	4494.442	
		C	-3.0230	-1.4441	-0.1381	728.9 733.4 763.1 775.4 795.3 844.7		
		C	-3.3532	-0.2856	-0.8525	861.6 872.8 888.8 942.1 954.3 978.5		
		C	-2.6079	0.8800	-0.6776	984.7 988.9 992.6 1025.2 1040.2		
		H	-1.1121	3.0620	0.2394	1041.5 1089.5 1123.0 1167.3 1177.1		
		H	-1.7522	-2.3035	1.3650	1178.4 1189.5 1220.6 1233.4 1270.7		
		H	-3.6143	-2.3442	-0.2656	1323.9 1329.7 1337.8 1427.9 1439.3		
		H	-4.1910	-0.2927	-1.5403	1461.7 1473.2 1514.2 1567.9 1578.3		
		H	-2.8632	1.7729	-1.2391	1603.5 1613.0 1649.3 3136.1 3146.0		

		C	-1.1827	-0.2663	0.9208	3150.6 3156.9 3158.3 3161.3 3165.0		
		H	-0.5749	-0.1671	1.8118	3168.8 3178.2 3182.5 3188.0		
		C	0.7079	2.0175	0.2740			
		H	1.2700	2.9466	0.2978			
		C	1.4989	0.7949	0.1105			
		C	2.8792	0.8581	-0.1687			
		C	0.9427	-0.4802	0.1574			
		C	3.6205	-0.3025	-0.3803			
		H	3.3653	1.8282	-0.2213			
		C	1.6377	-1.6484	-0.0402			
		C	3.0095	-1.5554	-0.3223			
		H	4.6813	-0.2293	-0.5919			
		H	1.1491	-2.6164	0.0132			
		H	3.5912	-2.4560	-0.4897			
TS15	-539.002357	C	-1.4206	0.8804	0.0092	-973.9 87.5 100.2 224.1 231.8 245.4	1134.703	2
		C	-0.6736	2.0982	0.0006	388.1 403.4 422.9 433.5 473.6 485.6	3293.984	
		C	-1.4989	-1.5718	0.0044	514.6 533.4 553.5 565.8 593.4 633.0	4396.659	
		C	-2.8689	-1.5271	-0.0888	710.7 726.1 729.8 748.7 764.6 805.9		
		C	-3.5478	-0.2908	-0.1002	825.2 840.0 877.9 880.5 891.4 957.7		
		C	-2.8278	0.8857	-0.0654	964.4 982.0 991.2 993.1 1013.7		
		H	-1.2184	3.0359	-0.0312	1052.7 1061.7 1112.2 1162.9 1170.8		
		H	-1.0032	-2.5332	0.0140	1184.9 1187.9 1223.4 1240.2 1261.1		
		H	-3.4323	-2.4503	-0.1647	1301.1 1313.0 1359.5 1364.1 1440.8		
		H	-4.6294	-0.2677	-0.1652	1441.9 1465.1 1484.0 1531.2 1549.6		
		H	-3.3408	1.8407	-0.1137	1593.9 1634.1 1642.7 1647.8 3156.7		
		C	-0.7240	-0.3757	0.1489	3159.8 3160.7 3169.6 3170.7 3176.2		
		H	-0.7142	-0.3475	1.9058	3184.0 3187.0 3194.4 3208.2		
		C	0.6855	2.0939	0.0165			
		H	1.2361	3.0286	0.0045			
		C	1.4316	0.8665	0.0075			
		C	2.8421	0.8807	-0.0579			
		C	0.7459	-0.3777	0.0458			
		C	3.5651	-0.2944	-0.0875			
		H	3.3523	1.8379	-0.0863			
		C	1.5078	-1.5605	0.0172			
		C	2.8895	-1.5241	-0.0509			
		H	4.6476	-0.2695	-0.1385			
		H	1.0161	-2.5239	0.0536			
		H	3.4509	-2.4512	-0.0740			
TS16	-540.138238	C	-1.9463	-0.2356	-0.0508	-1122.0 33.3 53.5 61.0 113.4 159.6	694.264	2
		C	-2.8429	-1.1438	-0.6389	181.3 260.2 323.5 354.0 366.0 411.7	7070.998	
		C	-4.2170	-0.9333	-0.5861	417.8 455.9 511.4 527.4 548.3 631.8	7394.624	
		C	-4.7275	0.1884	0.0655	634.4 650.5 701.2 704.8 756.5 768.8		
		C	-3.8510	1.0904	0.6696	832.3 846.5 848.7 852.2 865.1 927.8		
		C	-2.4770	0.8799	0.6194	933.3 981.5 983.0 990.6 998.0 999.5		
		H	-2.4518	-2.0175	-1.1500	1010.8 1014.8 1046.8 1049.4 1100.5		
		H	-4.8894	-1.6451	-1.0520	1102.7 1166.0 1177.7 1182.0 1182.6		
		H	-5.7980	0.3531	0.1122	1203.6 1205.6 1234.1 1292.8 1315.9		
		H	-4.2409	1.9561	1.1935	1344.2 1352.4 1360.9 1469.2 1477.1		
		H	-1.8117	1.5734	1.1173	1511.3 1525.5 1601.5 1612.1 1627.3		
		C	-0.5048	-0.4995	-0.1481	1637.9 1669.2 1813.7 3058.6 3157.1		
		H	-0.2443	-1.5324	-0.3952	3161.6 3165.2 3168.9 3175.1 3179.5		
		C	0.5084	0.3578	-0.0224	3185.1 3187.0 3191.6 3199.7		
		H	0.1876	1.7079	-0.0141			
		C	1.9437	0.1677	-0.0013			
		C	2.8027	1.0725	-0.6529			
		C	2.5157	-0.9205	0.6878			
		C	4.1789	0.8776	-0.6426			
		H	2.3794	1.9243	-1.1726			
		C	3.8929	-1.1130	0.6901			
		H	1.8696	-1.6042	1.2262			
		C	4.7301	-0.2168	0.0253			
		H	4.8248	1.5813	-1.1557			
		H	4.3156	-1.9584	1.2218			
		H	5.8040	-0.3646	0.0352			

		H	0.0201	2.5953	-0.0541			
TS17	-538.921195	C	-1.7100	-0.5407	0.0823	-590.4 30.5 52.7 69.6 123.0 220.2	903.061	2
		C	-2.8834	-1.2400	-0.2545	264.8 308.7 352.7 412.3 417.7 429.0	5475.171	
		C	-4.0921	-0.5745	-0.4301	508.5 562.2 588.9 619.5 631.9 666.8	6087.213	
		C	-4.1597	0.8095	-0.2757	699.5 726.3 747.8 756.7 802.7 813.2		
		C	-3.0030	1.5186	0.0565	821.4 848.8 865.4 905.1 921.1 955.1		
		C	-1.7950	0.8563	0.2331	977.7 979.0 991.4 1002.9 1011.4		
		H	-2.8389	-2.3173	-0.3789	1038.0 1046.9 1101.4 1121.7 1155.4		
		H	-4.9829	-1.1369	-0.6874	1180.1 1186.3 1196.1 1219.9 1251.8		
		H	-5.1005	1.3305	-0.4120	1276.4 1328.5 1352.1 1369.5 1423.0		
		H	-3.0461	2.5955	0.1790	1435.7 1477.7 1511.9 1523.3 1571.3		
		H	-0.9042	1.4159	0.4903	1609.0 1627.3 1717.2 3045.3 3136.4		
		C	-0.4621	-1.2836	0.2421	3154.9 3156.5 3162.2 3162.9 3172.5		
		H	-0.5419	-2.3660	0.1043	3173.8 3185.5 3188.4 3193.3		
		C	0.7478	-0.8147	0.5516			
		C	2.1199	-0.7742	0.6277			
		C	1.8571	0.6300	0.8519			
		C	3.2213	-1.2457	-0.0925			
		C	2.5946	1.5515	0.0243			
		H	1.4160	0.9752	1.7809			
		C	4.0576	-0.2972	-0.6691			
		H	3.3545	-2.3054	-0.2831			
		C	3.6824	1.0768	-0.6746			
		H	2.3622	2.6111	0.0295			
		H	4.9399	-0.6069	-1.2164			
		H	4.2890	1.7728	-1.2448			
TS18	-538.902533	C	-1.5025	0.8498	0.3246	-425.1 60.2 74.9 175.0 185.6 266.3	1404.765	2
		C	-2.7242	0.6715	-0.3629	309.9 395.3 405.0 460.6 476.4 501.3	2971.114	
		C	-3.1297	-0.5747	-0.7846	517.0 545.2 584.3 600.4 650.9 679.5	3717.452	
		C	-2.3200	-1.7209	-0.5201	712.0 735.8 747.9 753.4 788.9 806.2		
		C	-1.2099	-1.6236	0.2594	840.0 857.4 868.3 954.7 971.5 972.6		
		C	-0.7942	-0.3447	0.8502	983.4 987.8 1000.3 1013.6 1043.5		
		H	-3.2838	1.5539	-0.6579	1053.2 1144.6 1164.2 1168.1 1184.4		
		H	-4.0309	-0.6799	-1.3775	1196.7 1199.0 1216.8 1233.8 1277.5		
		H	-2.6176	-2.6836	-0.9215	1289.8 1336.4 1347.3 1361.5 1413.2		
		H	-0.6414	-2.5130	0.5081	1421.7 1450.7 1476.6 1504.7 1528.7		
		H	-0.9008	-0.3952	1.9351	1593.8 1626.7 1652.5 3041.9 3124.7		
		C	-0.8674	2.1307	0.3444	3133.7 3149.1 3153.1 3159.3 3165.9		
		H	-1.4803	3.0266	0.2858	3173.7 3175.1 3186.7 3189.1		
		C	0.4834	2.1673	0.1663			
		C	1.3499	1.1078	0.0968			
		C	1.0271	-0.0070	1.0173			
		C	2.3044	0.9152	-0.9458			
		C	1.8484	-1.2153	0.8675			
		C	2.9454	-0.2822	-1.0924			
		H	2.4865	1.7319	-1.6350			
		C	2.7217	-1.3528	-0.1593			
		H	1.7482	-2.0013	1.6097			
		H	3.6457	-0.4282	-1.9068			
		H	3.3033	-2.2633	-0.2585			
		H	0.9761	0.3253	2.0489			
TS19	-539.025240	C	-1.5290	0.8421	0.3223	-1326.9 74.9 92.8 154.5 205.2 273.1	1253.421	2
		C	-2.9107	0.6302	-0.0546	278.3 357.4 399.3 405.4 439.6 498.4	3058.652	
		C	-3.2736	-0.5614	-0.5881	513.1 529.9 573.6 593.7 609.3 661.5	3692.410	
		C	-2.2915	-1.6182	-0.8021	683.2 704.6 754.2 764.7 793.4 800.9		
		C	-1.0517	-1.5393	-0.2879	813.0 855.0 869.4 883.4 940.3 960.1		
		C	-0.7049	-0.3912	0.6303	974.6 976.5 988.2 989.7 1018.9		
		H	-3.6086	1.4599	-0.0128	1054.5 1070.0 1112.9 1124.3 1142.7		
		H	-4.2861	-0.7123	-0.9456	1165.2 1176.1 1190.5 1199.8 1212.5		
		H	-2.5781	-2.4732	-1.4054	1266.6 1293.9 1338.4 1347.5 1374.9		
		H	-0.3181	-2.3226	-0.4418	1390.0 1423.5 1437.0 1526.2 1573.7		
		H	-0.9820	-0.7277	1.6495	1589.2 1600.0 1667.2 1886.2 2873.6		
		C	-0.8682	2.0189	0.3918	3152.9 3153.5 3156.4 3160.7 3163.4		
		H	-1.3642	2.9816	0.3063	3171.2 3178.7 3185.7 3188.2		
		C	0.5929	1.9898	0.6483			
		C	1.2730	1.0406	-0.2245			
		C	0.7866	0.0218	0.7222			

		C	2.2986	0.8391	-1.1054			
		C	1.7887	-0.9885	1.0719			
		C	3.0479	-0.3456	-0.9325			
		H	2.6173	1.5991	-1.8109			
		C	2.8361	-1.1795	0.2032			
		H	1.6379	-1.6374	1.9288			
		H	3.8737	-0.5645	-1.5992			
		H	3.5311	-1.9928	0.3830			
		H	0.7083	1.0368	1.6319			
TS20	-538.936184	C	1.6147	0.0013	0.3159	-530.5 49.3 64.2 85.2 171.2 255.4	801.773	2
		C	2.4993	0.9669	0.8274	291.3 311.7 402.7 415.6 434.7 507.0	5709.934	
		C	3.8312	0.9979	0.4306	533.3 553.2 587.1 630.1 636.9 676.5	6005.915	
		C	4.3078	0.0634	-0.4898	701.5 716.5 747.5 765.6 783.6 850.9		
		C	3.4404	-0.8947	-1.0160	852.9 860.5 896.0 933.3 940.8 980.3		
		C	2.1059	-0.9197	-0.6257	982.3 985.9 1000.7 1014.4 1017.9		
		H	2.1320	1.6920	1.5465	1046.8 1097.4 1117.6 1148.9 1170.5		
		H	4.4998	1.7477	0.8387	1182.2 1197.9 1204.8 1233.3 1251.7		
		H	5.3460	0.0872	-0.8015	1306.2 1330.1 1351.1 1363.2 1428.4		
		H	3.8037	-1.6141	-1.7414	1447.4 1473.3 1492.4 1523.2 1568.1		
		H	1.4289	-1.6453	-1.0622	1597.2 1614.5 1635.8 3139.2 3151.8		
		C	0.2174	-0.0228	0.7535	3158.1 3162.7 3164.1 3172.0 3173.1		
		H	-0.0410	0.7414	1.4796	3178.5 3181.3 3182.2 3189.8		
		C	-0.6305	-1.1748	0.7018			
		H	-0.2851	-2.2016	0.6687			
		C	-1.9243	-0.6736	0.3616			
		C	-3.2526	-1.1361	0.3704			
		C	-1.6354	0.6024	-0.1468			
		C	-4.2337	-0.2871	-0.1344			
		H	-3.5102	-2.1194	0.7493			
		C	-2.5940	1.4630	-0.6374			
		C	-3.9185	0.9898	-0.6264			
		H	-5.2676	-0.6142	-0.1493			
		H	-2.3615	2.4493	-1.0238			
		H	-4.7123	1.6209	-1.0133			
TS21	-538.923771	C	-1.3964	0.3349	0.1733	-396.1 56.5 73.2 86.7 174.5 229.3	962.238	2
		C	-2.4983	0.9964	0.7560	260.3 305.8 400.4 414.8 441.6 492.5	4746.372	
		C	-3.7958	0.5512	0.5428	536.7 557.3 591.2 617.9 625.8 636.0	5317.001	
		C	-4.0300	-0.5650	-0.2633	679.3 699.9 737.2 754.8 778.0 807.2		
		C	-2.9541	-1.2242	-0.8614	838.7 843.9 851.2 864.4 906.5 931.5		
		C	-1.6550	-0.7777	-0.6547	953.9 980.6 986.9 999.6 1011.1		
		H	-2.3195	1.8634	1.3832	1017.1 1045.3 1104.8 1118.8 1158.8		
		H	-4.6280	1.0715	1.0037	1181.5 1186.0 1199.7 1232.3 1286.1		
		H	-5.0431	-0.9123	-0.4316	1325.3 1334.6 1353.9 1359.9 1419.3		
		H	-3.1330	-2.0811	-1.5013	1443.8 1477.6 1496.2 1518.7 1547.0		
		H	-0.8284	-1.2754	-1.1474	1589.3 1605.4 1627.2 3159.0 3159.7		
		C	-0.0546	0.8226	0.4105	3165.6 3170.7 3175.2 3179.4 3180.8		
		H	0.0278	1.7307	0.9942	3183.7 3185.2 3188.4 3192.0		
		C	1.5301	2.0456	-0.8372			
		H	1.8326	2.9440	-1.3641			
		C	2.1786	0.9705	-0.2786			
		C	3.5514	0.5744	-0.2479			
		C	1.1705	0.0863	0.2393			
		C	3.8392	-0.7290	0.0904			
		H	4.3326	1.2640	-0.5470			
		C	1.4827	-1.2559	0.5015			
		C	2.8133	-1.6479	0.4345			
		H	4.8671	-1.0747	0.0734			
		H	0.7191	-1.9553	0.8216			
		H	3.0840	-2.6675	0.6848			
TS22	-538.937317	C	-1.2928	0.6768	0.2448	-228.2 61.7 79.4 140.8 201.6 245.7	934.171	2
		C	-1.6047	-0.5991	0.7821	295.5 342.7 401.2 422.7 444.5 482.9	4337.196	
		C	-2.8623	-1.1825	0.5328	519.4 530.7 591.0 619.2 636.5 639.0	4985.038	
		C	-3.7980	-0.5219	-0.2451	712.2 715.2 723.9 744.7 762.3 801.6		
		C	-3.5166	0.7619	-0.7419	822.8 848.7 858.0 875.3 915.7 920.5		
		C	-2.2904	1.3548	-0.4863	959.5 972.8 982.7 988.3 1010.0		
		H	-1.0030	-0.9868	1.5926	1016.4 1040.9 1092.4 1135.4 1176.8		

		H	-3.0991	-2.1450	0.9722	1177.0 1191.1 1203.6 1222.2 1252.7		
		H	-4.7610	-0.9789	-0.4441	1327.8 1346.8 1375.6 1399.3 1429.7		
		H	-4.2599	1.2890	-1.3292	1466.3 1468.5 1509.2 1541.2 1578.1		
		H	-2.0726	2.3418	-0.8814	1594.7 1616.2 1656.1 3132.2 3157.0		
		C	0.0237	1.2507	0.3785	3157.9 3163.3 3164.1 3174.8 3177.6		
		H	0.0766	2.3362	0.4169	3183.9 3187.1 3189.7 3200.6		
		C	0.3226	-1.7275	-0.0097			
		H	0.2641	-2.7814	-0.2501			
		C	1.3465	-0.8559	-0.0663			
		C	2.6588	-1.3171	-0.5173			
		C	1.2246	0.5810	0.2935			
		C	3.7576	-0.5279	-0.4500			
		H	2.7364	-2.3434	-0.8577			
		C	2.4515	1.3445	0.3752			
		C	3.6568	0.8249	0.0309			
		H	4.7257	-0.9166	-0.7463			
		H	2.3771	2.3759	0.7037			
		H	4.5518	1.4331	0.0972			
TS23	-538.992668	C	1.2057	0.7429	0.0453	-1030.0 89.2 112.9 229.7 234.3 257.0	860.687	2
		C	1.2145	-0.7146	0.1552	369.8 383.8 394.5 457.6 472.9 488.8	4015.903	
		C	2.4780	-1.3992	-0.0438	512.6 541.2 556.3 590.0 616.5 638.0	4844.867	
		C	3.6397	-0.7001	-0.1451	659.9 736.2 742.1 761.6 766.6 780.7		
		C	3.6364	0.7300	-0.0915	816.7 834.0 863.5 891.7 908.9 915.2		
		C	2.4619	1.4224	-0.0094	927.6 969.7 976.5 990.1 994.2		
		H	1.3313	-0.7384	1.8586	1017.2 1029.8 1121.4 1152.4 1171.8		
		H	2.4732	-2.4832	-0.0749	1183.1 1189.2 1207.4 1273.3 1283.3		
		H	4.5805	-1.2233	-0.2735	1293.9 1326.0 1368.6 1403.5 1409.8		
		H	4.5784	1.2635	-0.1478	1420.5 1473.5 1476.6 1508.2 1566.4		
		H	2.4627	2.5075	-0.0127	1575.4 1611.6 1650.8 1662.7 3154.1		
		C	-0.0129	1.4110	0.0252	3158.0 3159.4 3161.0 3163.5 3166.1		
		H	-0.0190	2.4964	-0.0082	3175.8 3178.0 3187.9 3188.8		
		C	-0.0203	-1.4012	0.0259			
		H	-0.0148	-2.4862	0.0029			
		C	-1.2371	-0.7193	0.0016			
		C	-2.4918	-1.4019	-0.0572			
		C	-1.2390	0.7246	0.0235			
		C	-3.6711	-0.7078	-0.0762			
		H	-2.4915	-2.4867	-0.0790			
		C	-2.4895	1.4068	0.0035			
		C	-3.6714	0.7146	-0.0430			
		H	-4.6149	-1.2400	-0.1143			
		H	-2.4895	2.4918	0.0228			
		H	-4.6148	1.2484	-0.0572			
TS24	-538.811829	C	-1.4568	0.9353	0.1679	-425.1 60.2 74.9 175.0 185.6 266.3	1404.765	2
		C	-0.7983	-0.3421	0.2185	309.9 395.3 405.0 460.6 476.4 501.3	2971.114	
		C	-1.5135	-1.5351	-0.0230	517.0 545.2 584.3 600.4 650.9 679.5	3717.452	
		C	-2.8687	-1.4888	-0.2856	712.0 735.8 747.9 753.4 788.9 806.2		
		C	-3.5229	-0.2407	-0.3305	840.0 857.4 868.3 954.7 971.5 972.6		
		C	-2.8443	0.9421	-0.1120	983.4 987.8 1000.3 1013.6 1043.5		
		H	-0.2766	-0.2513	1.4408	1053.2 1144.6 1164.2 1168.1 1184.4		
		H	-1.0003	-2.4881	0.0002	1196.7 1199.0 1216.8 1233.8 1277.5		
		H	-3.4241	-2.4029	-0.4540	1289.8 1336.4 1347.3 1361.5 1413.2		
		H	-4.5865	-0.2086	-0.5424	1421.7 1450.7 1476.6 1504.7 1528.7		
		H	-3.3578	1.8944	-0.1655	1593.8 1626.7 1652.5 3041.9 3124.7		
		C	-0.6687	2.1019	0.3501	3133.7 3149.1 3153.1 3159.3 3165.9		
		C	0.7653	-0.2939	0.4899	3173.7 3175.1 3186.7 3189.1		
		H	0.7953	-0.0659	1.7667			
		C	1.4074	0.9364	-0.0661			
		C	2.7895	0.8832	-0.3572			
		C	0.6465	2.1165	-0.0546			
		C	3.5001	-0.2928	-0.3474			
		H	3.2803	1.8152	-0.6216			
		C	1.5025	-1.5555	0.2859			
		H	1.1366	3.0520	-0.3160			
		C	2.8148	-1.5139	-0.0711			

		H	4.5496	-0.3095	-0.6105			
		H	1.0188	-2.4989	0.4978			
		H	3.3491	-2.4521	-0.1847			
TS26	-540.157822	C	-1.1933	1.0490	-0.0362	-618.9 65.9 76.2 158.3 195.8 254.9	1565.177	2
		C	-0.3535	2.1184	-0.0790	317.1 353.2 380.6 428.7 447.2 500.7	2856.849	
		C	-1.7900	-1.2022	0.9053	512.8 519.8 581.5 599.0 611.6 675.0	3533.402	
		C	-2.7027	-1.3655	-0.0807	705.6 721.5 734.7 744.8 788.0 808.7		
		C	-2.9398	-0.3251	-1.0564	829.7 846.7 859.9 925.5 938.0 966.1		
		C	-2.2345	0.8321	-1.0180	971.7 980.3 984.6 991.8 1020.2		
		H	-0.4984	2.9032	-0.8145	1025.7 1037.8 1071.6 1108.4 1145.1		
		H	-1.6719	-1.9652	1.6687	1146.7 1161.3 1175.4 1184.3 1195.8		
		H	-3.3026	-2.2684	-0.1220	1200.7 1231.3 1279.6 1317.6 1329.4		
		H	-3.6941	-0.4811	-1.8193	1344.1 1378.7 1409.1 1445.0 1457.6		
		H	-2.4088	1.6109	-1.7539	1463.7 1481.5 1536.4 1548.4 1591.1		
		C	-0.9552	-0.0046	0.9903	1597.1 1660.9 2962.3 3026.3 3080.1		
		H	-0.9337	0.4114	1.9963	3086.6 3147.0 3147.6 3153.9 3157.6		
		C	0.9271	2.0985	0.7241	3160.8 3168.1 3173.5 3182.8 3188.1		
		H	0.7354	2.1965	1.8037			
		C	1.5526	0.7526	0.4160			
		C	2.4387	0.6038	-0.6299			
		C	0.9290	-0.4135	1.0302			
		C	2.7757	-0.6653	-1.1314			
		H	2.8612	1.4892	-1.0961			
		C	1.3061	-1.7071	0.4775			
		C	2.1737	-1.8148	-0.5810			
		H	3.4790	-0.7562	-1.9507			
		H	0.8892	-2.6023	0.9262			
		H	2.4222	-2.7930	-0.9785			
		H	1.5836	2.9203	0.4331			
		H	0.9355	-0.4031	2.1227			
TS27	-540.128166	C	-1.4819	0.8674	0.2056	-863.2 51.3 95.9 184.1 195.3 249.5	1227.718	2
		C	-0.8456	2.0309	0.0069	281.2 358.7 383.9 415.0 435.7 464.0	3307.965	
		C	-1.3781	-1.5842	-0.2459	493.5 506.1 547.2 551.4 569.1 615.1	4339.647	
		C	-2.6929	-1.5803	-0.5147	664.7 677.4 695.6 734.9 753.8 774.0		
		C	-3.5165	-0.4183	-0.2034	796.3 812.1 847.2 873.3 895.8 953.1		
		C	-2.9367	0.7576	0.1180	961.5 977.1 980.0 985.2 987.3 995.2		
		H	-1.4337	2.9335	-0.1404	1031.3 1055.9 1061.2 1128.4 1161.8		
		H	-0.7624	-2.4372	-0.5026	1182.9 1193.7 1202.0 1208.4 1209.9		
		H	-3.1569	-2.4353	-0.9952	1222.5 1266.7 1279.0 1289.1 1325.8		
		H	-4.5923	-0.4875	-0.3203	1372.8 1376.1 1398.4 1441.9 1458.9		
		H	-3.5302	1.6602	0.2248	1475.4 1505.0 1585.1 1596.0 1627.9		
		C	-0.7536	-0.4271	0.5181	1671.0 1706.5 2914.0 2957.9 3018.3		
		H	-0.9735	-0.6363	1.5800	3136.5 3152.4 3153.6 3160.9 3164.6		
		C	0.6418	2.1752	-0.0581	3176.4 3180.0 3188.3 3193.0		
		H	0.9902	2.7598	0.8086			
		C	1.3906	0.8661	-0.0808			
		C	2.7394	0.8468	-0.4324			
		C	0.7739	-0.3261	0.3859			
		C	3.4932	-0.3215	-0.3628			
		H	3.2096	1.7683	-0.7623			
		C	1.5472	-1.5168	0.3968			
		C	2.8881	-1.5097	0.0580			
		H	4.5403	-0.3103	-0.6427			
		H	1.0850	-2.4421	0.7212			
		H	3.4639	-2.4270	0.1081			
		H	0.9167	2.7750	-0.9343			
		H	1.0297	0.1178	2.1090			
TS28	-539.541382	C	-1.4412	0.8764	-0.0671	-1255.2 62.4 94.6 170.1 217.5 243.4	1187.323	1
		C	-0.7160	2.0865	-0.0534	278.2 377.9 410.2 436.6 438.8 483.6	3324.857	
		C	-1.5055	-1.5599	0.1820	491.1 533.0 547.6 554.6 576.0 636.0	4444.397	
		C	-2.9022	-1.5391	0.0337	646.9 692.6 703.6 723.6 747.1 750.2		
		C	-3.5605	-0.3409	-0.1954	789.9 817.6 848.1 864.3 872.9 920.5		
		C	-2.8287	0.8533	-0.2651	923.6 961.7 969.7 989.3 1000.6		
		H	-1.2496	3.0167	-0.2175	1039.3 1065.7 1075.1 1105.6 1135.4		
		H	-1.0194	-2.5137	0.3388	1181.0 1188.1 1192.3 1195.9 1216.9		

		H	-3.4556	-2.4703	0.0695	1256.6 1288.7 1297.9 1319.5 1342.9		
		H	-4.6356	-0.3232	-0.3323	1378.3 1427.0 1448.9 1470.2 1475.0		
		H	-3.3423	1.7912	-0.4483	1492.9 1523.1 1550.9 1578.0 1617.2		
		C	-0.7454	-0.3756	0.2173	1643.1 2921.4 2992.9 3152.1 3159.8		
		H	-0.6711	-0.0623	1.8605	3165.4 3168.0 3172.3 3183.2 3186.9		
		C	0.7497	2.1495	0.1964	3194.7 3207.0		
		H	0.9341	2.5590	1.2053			
		C	1.4604	0.8214	0.0677			
		C	2.8520	0.8040	-0.0646			
		C	0.7478	-0.3915	0.0863			
		C	3.5523	-0.3911	-0.1712			
		H	3.3900	1.7470	-0.0844			
		C	1.4670	-1.5907	-0.0340			
		C	2.8504	-1.5960	-0.1567			
		H	4.6316	-0.3845	-0.2727			
		H	0.9445	-2.5380	-0.0428			
		H	3.3786	-2.5382	-0.2494			
		H	1.2141	2.8782	-0.4817			
TS29	-539.010128	C	-1.4272	0.8478	-0.0515	-628.7 92.9 99.5 202.8 232.7 248.9	1152.670	2
		C	-0.6843	2.0663	-0.0950	297.7 347.5 408.8 423.2 437.8 446.6	3292.446	
		C	-1.5145	-1.5786	0.0641	507.1 513.1 548.8 558.0 600.7 631.7	4416.353	
		C	-2.8959	-1.5357	0.0494	722.2 725.7 730.6 751.5 767.4 798.0		
		C	-3.5690	-0.3038	-0.0215	840.5 842.7 874.1 880.9 887.8 958.3		
		C	-2.8418	0.8659	-0.0704	966.5 987.6 992.6 998.5 1016.6		
		H	-1.2274	3.0035	-0.1521	1060.3 1061.7 1113.3 1164.5 1168.1		
		H	-1.0279	-2.5436	0.1206	1182.4 1188.9 1222.6 1237.8 1264.0		
		H	-3.4623	-2.4591	0.0930	1304.8 1320.9 1364.4 1371.5 1441.3		
		H	-4.6526	-0.2760	-0.0338	1448.0 1463.4 1488.8 1528.8 1556.2		
		H	-3.3483	1.8241	-0.1202	1604.8 1618.4 1643.3 1650.9 3159.6		
		C	-0.7395	-0.4002	0.0105	3160.4 3164.2 3169.5 3170.8 3180.4		
		C	0.6845	2.0681	-0.0168	3183.3 3186.3 3193.0 3205.4		
		H	0.8820	2.5389	1.8992			
		C	1.4218	0.8268	-0.0206			
		C	2.8318	0.8310	-0.0434			
		C	0.7194	-0.4089	0.0030			
		C	3.5465	-0.3489	-0.0448			
		H	3.3499	1.7843	-0.0552			
		C	1.4790	-1.6002	0.0022			
		C	2.8600	-1.5741	-0.0207			
		H	4.6302	-0.3324	-0.0636			
		H	0.9795	-2.5601	0.0147			
		H	3.4152	-2.5053	-0.0219			
		H	1.2362	2.9919	-0.1467			
TS30	-540.087014	C	-1.5132	0.7992	0.4225	-463.5 78.5 90.0 158.1 180.7 239.2	1240.949	2
		C	-0.8822	1.9853	0.2155	257.5 296.2 329.4 379.9 401.0 433.7	3271.414	
		C	-1.2225	-1.5007	-0.4616	465.6 489.5 511.4 550.6 560.5 589.7	4141.810	
		C	-2.5298	-1.5197	-0.7731	645.9 687.4 698.1 716.5 737.7 762.9		
		C	-3.4372	-0.4995	-0.2630	784.2 816.8 829.8 873.7 900.4 924.1		
		C	-2.9488	0.6373	0.2917	944.0 966.1 976.5 976.7 981.6 988.1		
		H	-1.4769	2.8905	0.1359	994.3 1025.9 1068.7 1087.0 1120.0		
		H	-0.5346	-2.2378	-0.8584	1163.5 1175.8 1181.2 1200.8 1210.5		
		H	-2.9269	-2.2796	-1.4376	1236.9 1263.5 1269.2 1304.0 1330.9		
		H	-4.5010	-0.6051	-0.4439	1368.2 1382.3 1395.9 1408.8 1439.5		
		H	-3.6016	1.4777	0.5069	1459.0 1486.3 1561.9 1576.3 1622.9		
		C	-0.7392	-0.4948	0.5644	1665.3 1675.2 2896.7 2933.4 3150.3		
		H	-1.0511	-0.9265	1.5304	3151.2 3153.3 3156.8 3160.5 3170.6		
		C	0.5145	2.0531	-0.1392	3177.7 3178.8 3185.4 3187.9		
		H	0.9314	3.0056	-0.4442			
		C	1.3360	0.9572	-0.0098			
		C	2.6807	0.9202	-0.4906			
		C	0.7943	-0.2426	0.7481			
		C	3.4213	-0.2203	-0.4454			
		H	3.0850	1.8171	-0.9492			
		C	1.6339	-1.4819	0.6197			
		C	2.8673	-1.4494	0.0861			

		H	4.4286	-0.2307	-0.8457			
		H	1.2314	-2.4048	1.0254			
		H	3.4685	-2.3515	0.0440			
		H	0.2179	2.0902	-2.2601			
		H	0.8694	0.0688	1.8056			
TS31	-539.492844	C	-1.4185	0.9258	-0.0294	-2267.6 64.4 95.0 196.1 205.9 247.1	1195.270	1
		C	-0.6548	2.0963	-0.0129	364.2 374.9 413.8 431.2 460.9 482.7	3286.042	
		C	-1.5327	-1.5708	0.3047	494.9 534.2 567.5 580.1 652.2 680.8	4351.441	
		C	-2.8363	-1.5188	-0.0803	695.3 714.1 739.5 744.8 756.1 773.7		
		C	-3.5114	-0.2938	-0.3660	810.3 832.7 867.7 891.4 928.7 935.0		
		C	-2.7908	0.8763	-0.3601	959.1 963.3 973.6 978.9 997.4		
		H	-1.1583	3.0361	-0.2221	1017.6 1030.4 1049.6 1066.7 1120.3		
		H	-1.0599	-2.5178	0.5242	1159.7 1163.0 1180.5 1188.6 1237.0		
		H	-3.3726	-2.4543	-0.2069	1243.0 1266.2 1282.8 1353.2 1363.3		
		H	-4.5570	-0.3034	-0.6440	1405.2 1421.1 1452.7 1466.9 1494.4		
		H	-3.2695	1.8120	-0.6352	1542.8 1549.6 1580.5 1621.2 1639.6		
		C	-0.7873	-0.3132	0.5194	1665.2 1819.5 3147.2 3151.2 3155.4		
		H	-0.7984	-0.1003	1.8022	3161.8 3177.7 3184.4 3188.4 3196.6		
		C	0.7109	2.1078	0.2304	3200.1 3211.3		
		H	1.2567	3.0432	0.2364			
		C	1.4508	0.8926	0.1367			
		C	2.8467	0.8624	-0.1170			
		C	0.7788	-0.3732	0.1991			
		C	3.5122	-0.3292	-0.3100			
		H	3.3826	1.8028	-0.1831			
		C	1.4741	-1.5811	-0.0296			
		C	2.8317	-1.5653	-0.2759			
		H	4.5797	-0.3162	-0.5031			
		H	0.9435	-2.5236	-0.0007			
		H	3.3700	-2.4913	-0.4344			
		H	0.2431	-0.2811	1.4129			
TS32	-539.522326	C	-1.4327	0.9154	0.0195	-1039.3 60.7 97.1 190.9 201.2 248.1	1196.782	1
		C	-0.6428	2.1200	-0.0258	313.8 365.7 375.7 403.5 423.6 440.3	3318.544	
		C	-1.5575	-1.5756	0.3627	493.7 496.2 517.4 540.2 582.1 600.1	4420.028	
		C	-2.8599	-1.5393	-0.0615	656.2 683.9 718.6 723.7 760.8 768.9		
		C	-3.4902	-0.3274	-0.4031	804.5 823.9 833.6 857.8 887.2 924.7		
		C	-2.7477	0.8816	-0.3671	954.5 964.9 971.4 988.2 1012.1		
		H	-1.1490	3.0653	-0.1928	1017.0 1037.2 1064.9 1123.4 1131.5		
		H	-1.1169	-2.5218	0.6505	1150.9 1178.4 1186.1 1199.4 1214.0		
		H	-3.4168	-2.4671	-0.1425	1227.8 1237.4 1264.8 1308.1 1325.5		
		H	-4.5232	-0.3195	-0.7274	1335.3 1396.6 1420.2 1441.4 1479.9		
		H	-3.2245	1.8050	-0.6824	1509.7 1527.1 1559.9 1591.4 1620.4		
		C	-0.7490	-0.3258	0.5632	1638.1 2792.6 3151.7 3156.4 3158.7		
		C	0.7184	2.0883	0.1270	3159.6 3168.9 3172.3 3181.9 3187.3		
		H	0.9573	2.4919	1.9322	3195.1 3200.0		
		C	1.4432	0.8157	0.0639			
		C	2.8232	0.7910	-0.1777			
		C	0.7336	-0.3991	0.1795			
		C	3.5008	-0.4148	-0.3189			
		H	3.3606	1.7299	-0.2627			
		C	1.4229	-1.5997	0.0233			
		C	2.7971	-1.6129	-0.2244			
		H	4.5684	-0.4200	-0.5073			
		H	0.8967	-2.5434	0.0887			
		H	3.3120	-2.5595	-0.3432			
		H	1.2913	2.9935	-0.0410			
		H	-0.7129	-0.1592	1.6646			
TS33	-540.16704	C	-1.4061	0.1768	0.3471	-589.1 41.1 68.6 75.0 180.3 229.0	941.021	2
		C	-2.1337	0.9677	-0.5604	256.6 311.1 387.0 413.9 425.0 511.4	4908.719	
		C	-3.4638	0.6800	-0.8557	545.1 548.9 581.3 604.0 632.8 698.1	5352.205	
		C	-4.1024	-0.4049	-0.2569	703.5 706.8 765.0 778.2 804.9 819.5		
		C	-3.3947	-1.2029	0.6442	843.2 888.6 911.2 921.6 939.5 966.5		
		C	-2.0675	-0.9171	0.9393	977.2 992.0 993.7 1000.5 1006.0		
		H	-1.6632	1.8201	-1.0363	1016.1 1035.6 1049.2 1075.1 1099.5		
		H	-4.0047	1.3087	-1.5546	1152.7 1155.0 1166.0 1181.0 1187.1		

		H	-5.1386	-0.6250	-0.4865	1201.8 1231.0 1240.7 1303.4 1321.0		
		H	-3.8815	-2.0475	1.1196	1346.6 1352.1 1393.0 1437.7 1472.0		
		H	-1.5260	-1.5423	1.6420	1480.8 1483.7 1519.6 1526.7 1607.5		
		C	0.0147	0.4042	0.6465	1614.6 1631.1 3037.5 3054.1 3080.6		
		H	0.3567	-0.0993	1.5472	3130.8 3152.5 3155.4 3156.4 3161.9		
		C	0.7602	1.7336	0.4125	3171.9 3174.9 3180.2 3187.9 3189.1		
		H	0.9269	2.3473	1.3009			
		H	0.2749	2.3503	-0.3495			
		C	1.9496	0.9706	-0.1092			
		C	3.2428	0.9055	0.3293			
		C	1.2663	-0.1894	-0.6763			
		C	3.9751	-0.2977	0.1616			
		H	3.6835	1.7382	0.8690			
		C	2.0149	-1.4192	-0.7582			
		H	0.5594	-0.0060	-1.4877			
		C	3.3351	-1.4443	-0.3364			
		H	5.0110	-0.3498	0.4745			
		H	1.5588	-2.3047	-1.1865			
		H	3.8995	-2.3680	-0.4156			
TS34	-540.083395	C	1.0517	0.7074	-0.4896	-548.9 100.9 109.2 199.1 220.6 259.7	1153.266	2
		C	2.1860	1.3588	-0.0765	354.6 381.8 410.3 431.1 509.8 526.5	3159.822	
		C	3.3514	0.6305	0.2451	536.9 572.3 597.4 621.9 662.4 691.9	4050.877	
		C	3.3508	-0.7768	0.1755	713.4 740.3 772.0 804.1 832.0 858.4		
		C	2.2384	-1.4681	-0.2531	866.6 885.7 906.8 926.4 943.8 964.9		
		C	1.0003	-0.7844	-0.5775	972.4 979.7 988.8 1006.7 1021.1		
		H	2.1810	2.4389	0.0324	1023.2 1041.1 1063.9 1077.0 1095.4		
		H	4.2451	1.1564	0.5599	1147.0 1147.6 1165.6 1177.9 1182.0		
		H	4.2545	-1.3204	0.4300	1186.4 1207.4 1257.4 1308.2 1319.1		
		H	2.2829	-2.5472	-0.3627	1332.1 1354.3 1409.7 1413.4 1430.0		
		H	0.5132	-1.1593	-1.4814	1445.5 1466.5 1487.2 1534.9 1544.7		
		C	-0.3910	1.1207	-0.4777	1598.7 1660.2 3021.8 3033.9 3042.6		
		H	-0.8400	0.6391	-1.3517	3059.8 3110.9 3128.4 3138.7 3149.7		
		C	-1.4645	2.2059	-0.0702	3152.2 3154.8 3164.5 3168.1 3186.1		
		H	-1.9341	2.7789	-0.8687			
		H	-1.1396	2.8623	0.7399			
		C	-2.1804	0.9263	0.4313			
		C	-3.1468	0.1451	-0.0874			
		C	-0.8640	0.3061	0.7701			
		C	-2.8965	-1.2978	-0.1658			
		H	-4.0147	0.5521	-0.5969			
		C	-0.5184	-1.1349	0.5786			
		H	-0.3997	0.7657	1.6472			
		C	-1.6852	-1.8804	0.0648			
		H	-3.7142	-1.9304	-0.4984			
		H	-0.0277	-1.6307	1.4128			
		H	-1.5963	-2.9551	-0.0677			
TS35	-540.042337	C	1.0227	0.7515	-0.1305	-686.5 111.0 127.1 215.6 252.9 260.6	1139.614	2
		C	2.2350	1.3745	-0.3486	358.5 372.9 387.1 424.5 432.8 485.8	3159.792	
		C	3.4169	0.6193	-0.2793	496.5 508.3 548.1 564.8 606.9 652.2	4011.688	
		C	3.3760	-0.7421	0.0173	679.5 707.5 746.0 753.4 775.9 826.0		
		C	2.1568	-1.3856	0.2370	843.6 863.0 886.8 899.0 928.8 951.7		
		C	0.9596	-0.6701	0.1081	954.4 981.6 987.8 991.2 991.5		
		H	2.2793	2.4376	-0.5581	1014.6 1033.9 1040.3 1073.7 1092.1		
		H	4.3725	1.1060	-0.4396	1136.8 1152.5 1162.9 1179.8 1180.9		
		H	4.3006	-1.3029	0.0961	1187.5 1207.6 1251.4 1275.5 1308.5		
		H	2.1358	-2.4403	0.4914	1318.4 1335.2 1337.9 1404.6 1423.2		
		H	0.6163	-1.1625	-1.7196	1443.3 1449.5 1482.7 1486.9 1586.0		
		C	-0.4329	1.1741	-0.2048	1590.4 1624.1 1674.5 2996.3 3008.0		
		H	-0.7454	0.7497	-1.1664	3033.5 3059.9 3130.3 3140.1 3153.4		
		C	-1.6227	2.1818	0.1079	3157.6 3164.9 3165.6 3175.1 3186.6		
		H	-2.0041	2.7848	-0.7150			
		H	-1.4624	2.7926	0.9988			
		C	-2.3247	0.8230	0.4087			
		C	-3.1257	0.0223	-0.3139			
		C	-1.0259	0.2728	0.8914			

		C	-2.6974	-1.3741	-0.5240			
		H	-3.9358	0.4051	-0.9271			
		C	-0.4610	-1.1060	0.6275			
		H	-0.7309	0.6858	1.8616			
		C	-1.4646	-1.8553	-0.2377			
		H	-3.3773	-2.0189	-1.0734			
		H	-0.3112	-1.6901	1.5431			
		H	-1.2101	-2.8646	-0.5461			
TS36	-539.458966	C	0.8379	0.7612	0.1280	-147.0 -55.0 79.6 132.1 157.9 213.9	1329.228	1
		C	1.9944	1.4068	-0.3497	270.3 299.7 376.8 390.9 413.3 459.5	2758.708	
		C	3.1533	0.6724	-0.4966	490.1 499.9 528.5 536.7 548.2 591.6	3509.761	
		C	3.1761	-0.7122	-0.2323	648.1 707.5 725.5 738.9 758.6 796.7		
		C	2.0301	-1.3680	0.2107	808.5 835.3 863.5 894.0 933.2 943.6		
		C	0.8683	-0.6337	0.4188	951.8 969.8 979.1 984.1 988.5		
		H	1.9512	2.4501	-0.6344	1029.8 1037.4 1074.2 1083.5 1106.2		
		H	4.0547	1.1601	-0.8497	1131.8 1157.9 1170.5 1175.2 1184.4		
		H	4.0936	-1.2699	-0.3812	1197.6 1237.9 1281.3 1304.4 1310.1		
		H	2.0529	-2.4351	0.4058	1327.4 1363.5 1385.9 1411.3 1463.1		
		C	-0.4418	1.2728	0.5121	1467.8 1489.1 1545.7 1580.2 1618.0		
		H	-0.2892	2.1235	-2.2302	1651.3 2983.7 3016.8 3053.9 3151.5		
		C	-1.6400	2.1558	0.1970	3159.8 3170.0 3170.6 3182.1 3184.4		
		H	-1.6123	2.7852	-0.6810	3185.6 3196.8		
		H	-2.0348	2.6436	1.0990			
		C	-2.1498	0.7144	0.0629			
		C	-2.5683	-0.0778	-0.9489			
		C	-1.2439	0.1800	1.1537			
		C	-2.2164	-1.4878	-0.9250			
		H	-3.0299	0.3350	-1.8376			
		C	-0.4985	-1.1317	0.9070			
		H	-1.6037	0.3811	2.1676			
		C	-1.2336	-1.9703	-0.1349			
		H	-2.6825	-2.1456	-1.6508			
		H	-0.3933	-1.7195	1.8223			
		H	-0.9127	-3.0008	-0.2468			
TS37	-538.922034	C	0.8649	0.7671	0.2033	-619.6 84.7 100.5 191.9 220.5 245.2	1432.987	2
		C	2.0605	1.2711	-0.3263	351.4 390.7 440.6 472.5 495.4 529.5	2579.66	
		C	3.1137	0.3945	-0.5676	547.9 555.5 596.2 623.1 695.5 707.7	3415.113	
		C	2.9792	-0.9702	-0.2910	725.6 753.8 766.4 784.8 809.0 821.5		
		C	1.7843	-1.4783	0.2279	867.8 876.3 912.1 935.8 945.5 954.1		
		C	0.7310	-0.6110	0.4826	967.6 970.0 988.1 994.3 1041.2		
		H	2.1683	2.3310	-0.5294	1056.5 1096.9 1130.4 1165.8 1179.2		
		H	4.0480	0.7713	-0.9685	1180.1 1192.1 1223.7 1243.9 1279.8		
		H	3.8106	-1.6401	-0.4802	1290.8 1318.5 1320.4 1351.5 1392.9		
		H	1.6872	-2.5407	0.4248	1416.6 1482.6 1488.1 1501.3 1541.3		
		C	-0.3554	1.4581	0.5458	1605.0 1623.9 1649.4 3031.5 3049.4		
		C	-1.0008	2.5472	-0.0281	3115.6 3142.9 3159.5 3165.6 3167.0		
		H	-0.5295	3.1338	-0.8139	3173.2 3176.4 3187.6 3212.3		
		H	-1.8208	3.0307	0.4861			
		C	-2.1733	0.7742	-0.1888			
		C	-2.3934	-0.1044	-1.1824			
		C	-1.3704	0.4509	1.0449			
		C	-2.1920	-1.5247	-0.8802			
		H	-2.7626	0.1933	-2.1571			
		C	-0.6652	-0.9393	1.0186			
		H	-1.8696	0.6879	1.9877			
		C	-1.4132	-1.9303	0.1390			
		H	-2.6930	-2.2602	-1.5031			
		H	-0.5843	-1.3490	2.0304			
		H	-1.2731	-2.9880	0.3357			
TS38	-538.902739	C	1.1240	0.6712	0.0132	-1612.5 65.2 105.9 134.1 192.9 253.7	1284.200	2
		C	2.4570	0.9930	-0.2527	277.8 386.1 393.2 421.7 448.7 500.3	3075.059	
		C	3.4117	-0.0202	-0.2617	520.3 541.6 557.7 590.2 631.3 671.3	4200.862	
		C	3.0451	-1.3449	-0.0045	707.2 719.9 742.3 749.5 769.4 790.8		
		C	1.7154	-1.6699	0.2669	814.4 849.0 882.3 898.5 906.0 954.9		
		C	0.7591	-0.6601	0.2704	959.1 970.5 992.0 1005.5 1020.3		

		H	2.7498	2.0177	-0.4525	1044.6 1077.7 1114.8 1124.2 1156.7		
		H	4.4486	0.2191	-0.4692	1180.2 1191.3 1212.0 1222.7 1263.9		
		H	3.7995	-2.1235	-0.0138	1278.7 1325.3 1340.2 1361.2 1386.5		
		H	1.4372	-2.6983	0.4726	1413.8 1437.6 1492.4 1498.5 1593.8		
		C	-0.0578	1.5547	0.0547	1616.9 1640.8 1665.7 2073.6 2938.1		
		C	-0.1106	2.8739	-0.1824	3144.7 3145.8 3159.2 3166.5 3167.6		
		H	0.7793	3.4443	-0.4194	3174.3 3177.3 3188.4 3230.7		
		H	-1.0515	3.4097	-0.1451			
		C	-2.5809	0.9155	0.1360			
		C	-3.4426	-0.1377	-0.0583			
		C	-1.2114	0.6670	0.3800			
		C	-2.8574	-1.3564	-0.5932			
		H	-4.5138	-0.0572	0.0866			
		C	-0.7248	-0.7745	0.5632			
		C	-1.5657	-1.6674	-0.3372			
		H	-3.4672	-2.0284	-1.1899			
		H	-0.8548	-1.1187	1.6024			
		H	-1.1229	-2.5828	-0.7158			
		H	-1.9704	1.2529	1.2782			
TS39	-538.931764	C	-1.1737	0.7505	-0.1941	-884.5 80.3 104.8 162.8 207.4 225.6	1222.985	2
		C	-2.5096	1.0434	-0.4731	316.1 387.3 405.7 440.0 459.2 466.8	3127.183	
		C	-3.4565	0.0217	-0.3906	523.9 560.5 585.1 607.3 646.3 695.3	4109.549	
		C	-3.0796	-1.2722	-0.0246	713.5 731.8 765.5 768.5 791.2 818.8		
		C	-1.7453	-1.5621	0.2833	845.9 883.1 932.4 949.9 951.3 958.4		
		C	-0.7978	-0.5530	0.1949	973.5 980.9 986.5 1022.3 1037.3		
		H	-2.8019	2.0438	-0.7726	1047.2 1107.5 1142.0 1152.4 1174.5		
		H	-4.4950	0.2328	-0.6205	1178.8 1184.2 1206.5 1220.7 1246.5		
		H	-3.8263	-2.0564	0.0270	1282.8 1310.6 1339.7 1374.4 1418.4		
		H	-1.4665	-2.5640	0.5931	1457.5 1482.5 1486.4 1493.3 1516.3		
		C	0.0069	1.6136	-0.2556	1607.2 1631.8 1645.7 2861.8 3065.0		
		C	0.4442	2.4416	0.7867	3153.1 3156.8 3158.9 3164.4 3172.9		
		H	-0.1281	2.5883	1.7049	3175.8 3186.3 3186.5 3188.1		
		H	1.3328	3.0528	0.6794			
		C	2.5462	0.8944	-0.3681			
		C	3.3417	-0.2148	-0.4742			
		C	1.1958	0.7699	0.0473			
		C	2.8045	-1.5395	-0.2396			
		H	4.3626	-0.1150	-0.8231			
		C	0.6747	-0.5633	0.6008			
		C	1.5503	-1.7297	0.2137			
		H	3.4348	-2.3962	-0.4544			
		H	0.6867	-0.5253	1.7075			
		H	1.1691	-2.7289	0.3956			
		H	2.9202	1.8649	-0.6772			
TS40	-538.876059	C	1.1321	0.7977	-0.2536	-1876.8 69.6 98.1 175.1 219.1 268.2	1193.789	2
		C	2.4195	1.0616	-0.7040	326.7 381.6 393.8 448.6 454.3 484.8	3098.256	
		C	3.3974	0.0721	-0.5620	523.0 566.1 579.2 604.7 633.3 663.2	3865.154	
		C	3.0864	-1.1526	0.0250	712.6 740.5 747.1 767.1 797.0 812.2		
		C	1.7871	-1.4114	0.4786	831.4 861.7 874.6 916.5 949.8 954.5		
		C	0.8061	-0.4422	0.3265	962.0 972.1 985.0 986.1 992.2		
		H	2.6611	2.0160	-1.1577	1042.5 1045.2 1096.7 1121.4 1156.2		
		H	4.4057	0.2609	-0.9130	1177.9 1188.9 1200.4 1211.0 1231.5		
		H	3.8521	-1.9134	0.1256	1254.2 1295.3 1311.5 1337.5 1371.1		
		H	1.5546	-2.3686	0.9345	1412.7 1445.7 1482.0 1487.4 1614.4		
		C	-0.0804	1.6300	-0.2201	1632.7 1639.1 1701.3 2261.9 2952.4		
		C	-0.7425	2.0309	1.0560	3150.3 3156.3 3161.4 3166.2 3166.8		
		H	-0.2570	2.1510	2.0173	3172.4 3177.9 3183.6 3188.4		
		C	-2.6112	0.8534	-0.3305			
		C	-3.2116	-0.2869	-0.6999			
		C	-1.2773	0.8540	0.3129			
		C	-2.5755	-1.5845	-0.4725			
		H	-4.1814	-0.2628	-1.1845			
		C	-0.6686	-0.5143	0.7484			
		C	-1.4113	-1.6997	0.1782			
		H	-3.0754	-2.4738	-0.8419			

		H	-0.6996	-0.6083	1.8457			
		H	-0.9706	-2.6770	0.3464			
		H	-3.0728	1.8188	-0.5068			
		H	-0.5172	2.8092	0.0365			
TS41	-538.949117	C	-1.3419	0.8080	0.4127	-425.8 75.1 101.3 170.8 225.3 282.8	1228.157	2
		C	-0.7653	2.0190	0.9912	361.9 378.6 426.1 465.1 473.8 486.2	3073.150	
		C	-1.3859	-1.7176	0.1157	533.5 567.6 589.6 602.6 675.3 706.1	3917.545	
		C	-2.5735	-1.6072	-0.5035	737.8 757.7 770.9 777.1 797.9 853.7		
		C	-3.2140	-0.3206	-0.6830	860.2 876.4 901.6 952.7 954.4 959.9		
		C	-2.6012	0.8261	-0.2787	982.0 984.2 986.8 1032.9 1049.9		
		H	-1.3687	2.9169	1.0883	1071.3 1121.9 1144.7 1178.5 1186.1		
		H	-0.9070	-2.6853	0.2201	1193.2 1197.7 1221.0 1233.0 1241.6		
		H	-3.0618	-2.4914	-0.8995	1284.3 1292.6 1324.9 1340.2 1375.5		
		H	-4.1812	-0.2761	-1.1700	1416.0 1460.6 1484.1 1505.9 1526.8		
		H	-3.0702	1.7893	-0.4524	1615.1 1631.2 1665.3 2923.8 3093.3		
		C	-0.6803	-0.5336	0.7312	3141.2 3153.7 3157.8 3159.3 3164.1		
		H	-0.7268	-0.6550	1.8284	3173.8 3175.7 3185.8 3188.2		
		C	0.1156	1.8711	-0.1233			
		H	0.1522	2.6377	-0.8982			
		C	1.1482	0.8254	-0.1587			
		C	2.4468	1.0387	-0.6317			
		C	0.7950	-0.4248	0.3688			
		C	3.3917	0.0179	-0.5411			
		H	2.7232	2.0022	-1.0465			
		C	1.7467	-1.4302	0.4838			
		C	3.0475	-1.2097	0.0239			
		H	4.3991	0.1830	-0.9061			
		H	1.4802	-2.3951	0.9023			
		H	3.7846	-2.0018	0.0909			
TS42	-540.141958	C	1.6133	-0.1765	0.9436	-447.9 19.3 42.7 66.6 116.4 167.5	965.728	2
		C	1.8271	1.1705	0.7802	270.8 324.7 359.5 403.4 413.6 484.5	4974.307	
		C	3.0311	1.5803	0.1664	524.8 553.5 579.6 591.9 635.8 640.5	5549.409	
		C	3.8059	0.6187	-0.5229	709.2 711.8 740.3 765.3 780.2 816.6		
		C	3.5307	-0.7358	-0.4709	837.3 854.2 871.8 910.5 928.9 949.7		
		C	2.4898	-1.1904	0.4287	969.3 971.5 982.6 999.3 1004.7		
		H	1.0528	1.8919	1.0233	1016.3 1017.7 1049.3 1086.7 1106.7		
		H	3.2966	2.6290	0.1085	1130.0 1147.5 1178.9 1181.0 1195.8		
		H	4.6491	0.9604	-1.1157	1202.3 1211.4 1272.2 1314.9 1334.8		
		H	4.1502	-1.4469	-1.0063	1344.5 1357.6 1379.9 1422.9 1448.6		
		H	2.6339	-2.1297	0.9576	1478.7 1482.7 1517.0 1523.9 1622.3		
		C	0.6863	-1.1648	0.4256	1631.9 1640.9 3015.8 3073.6 3096.3		
		H	0.3969	-2.0018	1.0563	3120.0 3149.4 3150.6 3152.4 3157.2		
		C	-0.1636	-0.9205	-0.8002	3167.3 3170.7 3175.1 3187.0 3187.2		
		H	-0.2864	-1.8651	-1.3423			
		H	0.3604	-0.2273	-1.4635			
		C	-1.5355	-0.3632	-0.4551			
		C	-2.5696	-1.2156	-0.0512			
		C	-1.7900	1.0109	-0.5120			
		C	-3.8212	-0.7096	0.2933			
		H	-2.3953	-2.2866	-0.0120			
		C	-3.0413	1.5214	-0.1701			
		H	-1.0034	1.6855	-0.8338			
		C	-4.0609	0.6627	0.2367			
		H	-4.6105	-1.3869	0.6006			
		H	-3.2209	2.5896	-0.2261			
		H	-5.0351	1.0582	0.5013			
TS43	-540.075126	C	1.5673	0.1909	0.5937	-467.3 26.2 32.5 70.3 121.0 162.4	914.263	2
		C	2.1763	1.4271	0.6115	181.7 252.1 329.1 347.5 379.5 409.1	5346.108	
		C	3.5184	1.4062	0.1846	413.8 471.9 505.7 520.9 572.2 621.8	5908.919	
		C	4.1240	0.2391	-0.3087	636.0 681.2 712.2 723.8 750.0 758.1		
		C	3.4375	-0.9830	-0.3839	816.1 851.9 854.3 893.9 929.2 937.6		
		C	2.1618	-0.9555	0.1684	963.7 981.5 994.4 998.5 1011.9 1016.2		
		H	1.6926	2.3510	0.9083	1017.3 1025.0 1049.8 1079.4 1103.4		
		H	4.0960	2.3242	0.2031	1123.4 1129.6 1176.5 1180.9 1194.7		
		H	5.1500	0.2928	-0.6569	1202.6 1220.7 1293.1 1315.3 1336.9		

		H	3.9037	-1.8671	-0.8040	1353.4 1366.1 1377.4 1464.6 1475.9		
		H	2.6218	-2.1493	1.7903	1482.8 1487.7 1525.6 1585.2 1622.6		
		C	0.6586	-0.9768	0.3802	1642.9 1700.2 3029.0 3067.8 3083.9		
		H	0.3048	-1.5045	1.2660	3151.8 3155.8 3157.8 3166.8 3167.0		
		C	-0.3276	-1.0324	-0.7893	3175.2 3175.6 3184.4 3187.2		
		H	-0.4588	-2.0820	-1.0733			
		H	0.1093	-0.5175	-1.6490			
		C	-1.6684	-0.4241	-0.4402			
		C	-1.9268	0.9289	-0.6868			
		C	-2.6673	-1.1917	0.1693			
		C	-3.1478	1.5003	-0.3330			
		H	-1.1665	1.5383	-1.1647			
		C	-3.8891	-0.6242	0.5264			
		H	-2.4895	-2.2456	0.3604			
		C	-4.1331	0.7252	0.2766			
		H	-3.3311	2.5495	-0.5372			
		H	-4.6519	-1.2369	0.9942			
		H	-5.0844	1.1676	0.5499			
TS44	-540.053163	C	-1.6161	0.2514	-0.4370	-869.1 25.5 31.5 64.7 104.6 161.2	923.563	2
		C	-2.3097	1.4327	-0.5946	181.9 235.0 259.3 332.9 346.9 389.1	5483.993	
		C	-3.6829	1.3238	-0.2956	418.5 447.3 515.7 516.0 571.2 620.3	6047.835	
		C	-4.2617	0.1194	0.1283	623.4 680.9 705.5 726.4 747.4 752.2		
		C	-3.5087	-1.0622	0.2827	813.5 842.5 869.4 895.9 915.4 935.5		
		C	-2.1743	-0.9097	-0.0300	949.3 957.1 975.6 987.4 991.4		
		H	-1.8745	2.3721	-0.9169	1006.1 1017.9 1027.3 1029.4 1057.3		
		H	-4.3169	2.1984	-0.3953	1083.4 1124.2 1126.1 1137.5 1176.3		
		H	-5.3248	0.1007	0.3436	1177.2 1191.4 1215.2 1295.1 1297.5		
		H	-3.9694	-1.9852	0.6167	1314.7 1326.7 1361.4 1384.3 1452.5		
		C	-0.6961	-0.9303	-0.3084	1471.3 1477.9 1480.3 1487.2 1580.5		
		H	-0.3633	-1.4077	-1.2322	1602.7 1629.7 1725.4 2329.1 3038.4		
		C	0.3366	-1.0404	0.8180	3057.4 3085.7 3151.4 3156.5 3159.7		
		H	0.4899	-2.1008	1.0404	3166.0 3171.3 3174.7 3183.5		
		H	-0.0678	-0.5727	1.7191			
		C	1.6568	-0.3982	0.4530			
		C	2.6332	-1.0557	-0.2779			
		C	1.9498	0.9295	0.8069			
		C	3.8380	-0.5099	-0.6679			
		H	2.4125	-2.4865	-0.6513			
		C	3.1542	1.5257	0.4347			
		H	1.2233	1.4939	1.3839			
		C	4.1009	0.8150	-0.3024			
		H	4.5616	-1.0862	-1.2348			
		H	3.3559	2.5506	0.7255			
		H	5.0377	1.2813	-0.5879			
		H	2.3161	-3.3051	-0.8690			
TS45	-538.888662	C	-2.0372	0.8717	0.3685	-384.4 50.3 88.2 175.9 198.5 234.8	1431.818	2
		C	-2.2824	-0.0287	1.3992	267.5 371.4 431.2 461.5 470.7 479.1	2816.041	
		C	-2.2464	-1.3810	1.0002	497.7 563.9 598.8 639.8 677.0 696.3	3514.188	
		C	-1.7913	-1.7694	-0.2614	725.6 742.6 753.8 772.0 854.8 863.1		
		C	-1.3083	-0.8084	-1.2049	879.1 892.6 932.0 960.6 972.3 982.6		
		C	-1.6871	0.5054	-0.8799	990.1 996.5 1010.2 1020.6 1050.3		
		H	-2.4892	0.2498	2.4262	1064.5 1107.2 1124.4 1146.9 1172.1		
		H	-2.5296	-2.1520	1.7097	1177.0 1200.9 1229.1 1249.7 1277.7		
		H	-1.7240	-2.8260	-0.4954	1302.7 1321.1 1355.5 1374.9 1447.3		
		H	-0.9995	-1.1209	-2.1959	1453.5 1467.1 1471.4 1481.0 1543.3		
		C	-1.2641	1.8743	-0.4661	1577.7 1623.9 1671.1 3006.2 3043.5		
		H	-1.8043	2.7292	-0.8692	3088.3 3140.5 3148.7 3154.8 3164.1		
		C	0.2208	2.1305	-0.2266	3164.8 3174.5 3181.4 3182.7		
		H	0.3521	2.7686	0.6540			
		H	0.5945	2.7115	-1.0793			
		C	1.0889	0.8870	-0.0848			
		C	0.7713	-0.3672	-0.5904			
		C	2.3478	0.9987	0.5338			
		C	1.6031	-1.4672	-0.5201			
		C	3.2198	-0.0839	0.6129			

		H	2.6442	1.9569	0.9523			
		C	2.8560	-1.3212	0.0817			
		H	1.2944	-2.4304	-0.9146			
		H	4.1833	0.0375	1.0952			
		H	3.5325	-2.1673	0.1438			
TS46	-538.912151	C	2.6770	0.8120	0.1260	-413.4 34.9 101.7 183.0 224.2 265.0	1242.028	2
		C	3.1074	-0.1806	-0.8027	335.1 389.8 420.7 440.4 461.0 487.1	3037.460	
		C	2.5142	-1.4707	-0.7450	519.0 535.5 569.4 630.1 680.5 701.0	3869.828	
		C	1.4024	-1.7393	0.0100	718.7 742.2 759.0 770.5 797.0 829.5		
		C	0.7062	-0.6753	0.8392	868.8 877.7 919.8 939.6 965.7 971.5		
		C	1.5321	0.5671	0.8051	991.3 991.9 1015.9 1037.7 1065.9		
		H	3.8818	0.0236	-1.5346	1121.0 1145.8 1177.9 1186.6 1188.6		
		H	2.9377	-2.2726	-1.3447	1197.8 1206.5 1222.1 1234.1 1264.4		
		H	0.9718	-2.7344	0.0032	1308.7 1325.2 1339.0 1356.8 1417.4		
		H	0.6445	-1.0421	1.8770	1436.3 1461.5 1477.3 1514.6 1522.0		
		C	1.1030	1.8773	0.5398	1589.2 1615.8 1641.9 2939.7 2993.0		
		H	1.6418	2.7352	0.9078	3025.3 3135.1 3150.1 3155.2 3159.6		
		C	-0.2085	2.0717	-0.1707	3171.9 3175.5 3187.0 3240.4		
		H	-0.0188	2.3398	-1.2196			
		H	-0.7250	2.9384	0.2586			
		C	-1.1313	0.8611	-0.1077			
		C	-0.7330	-0.3957	0.3790			
		C	-2.4568	1.0276	-0.5335			
		C	-1.6725	-1.4334	0.4401			
		C	-3.3765	-0.0118	-0.4826			
		H	-2.7685	1.9986	-0.9068			
		C	-2.9822	-1.2539	0.0144			
		H	-1.3693	-2.3983	0.8343			
		H	-4.3949	0.1469	-0.8187			
		H	-3.6909	-2.0720	0.0746			
TS47	-538.875305	C	2.6830	0.8732	-0.1129	-1999.4 34.5 75.8 146.4 203.0 250.3	1264.793	2
		C	3.1503	-0.1888	-0.8536	336.3 387.2 397.1 439.9 462.0 484.7	3052.976	
		C	2.6256	-1.4981	-0.5224	516.0 522.7 535.5 594.4 640.2 688.2	3981.553	
		C	1.5172	-1.6807	0.2397	708.4 727.6 750.4 779.8 803.3 820.5		
		C	0.7343	-0.5332	0.8591	863.2 870.5 905.7 917.9 955.6 962.7		
		C	1.4761	0.7346	0.6171	989.1 991.8 1003.1 1029.4 1058.4		
		H	3.8862	-0.0808	-1.6416	1071.0 1117.2 1179.4 1184.4 1190.0		
		H	3.1321	-2.3731	-0.9205	1193.1 1199.2 1217.0 1233.7 1246.8		
		H	1.1789	-2.6898	0.4467	1277.3 1317.9 1336.4 1348.9 1397.9		
		H	0.6771	-0.7285	1.9421	1418.3 1436.6 1474.5 1511.7 1573.9		
		C	0.9924	1.9834	0.4016	1599.1 1612.3 1639.0 1903.2 2949.2		
		H	2.2659	2.2343	-0.1472	2996.6 3026.7 3142.6 3149.1 3161.2		
		C	-0.4442	2.1751	0.0424	3171.7 3176.3 3181.7 3187.3		
		H	-0.5119	2.6944	-0.9214			
		H	-0.9091	2.8632	0.7619			
		C	-1.2454	0.8695	-0.0117			
		C	-0.7216	-0.3805	0.3623			
		C	-2.5776	0.9411	-0.4415			
		C	-1.5483	-1.5095	0.3065			
		C	-3.3872	-0.1863	-0.5004			
		H	-2.9828	1.9058	-0.7327			
		C	-2.8683	-1.4228	-0.1194			
		H	-1.1525	-2.4745	0.6036			
		H	-4.4139	-0.1017	-0.8385			
		H	-3.4872	-2.3124	-0.1528			
TS48	-538.916432	C	2.6036	0.8768	-0.5931	49.0 93.5 205.0 211.6 247.9 373.9	1168.140	2
		C	3.2713	-0.3399	-0.7139	388.2 414.3 429.0 485.0 487.0 519.1	3282.737	
		C	2.7528	-1.5064	-0.0740	543.9 565.0 602.6 665.6 687.5 716.3	4379.292	
		C	1.5951	-1.4726	0.6314	723.1 745.8 779.6 804.7 819.9 832.1		
		C	0.7710	-0.2221	0.7589	863.5 887.0 934.0 952.5 962.7 967.3		
		C	1.3974	0.9922	0.0893	976.7 986.0 1008.7 1045.9 1065.4		
		H	4.1984	-0.4002	-1.2710	1124.5 1132.4 1157.0 1181.9 1188.8		
		H	3.3144	-2.4330	-0.1365	1200.0 1215.9 1233.6 1248.8 1272.4		
		H	1.2559	-2.3584	1.1575	1306.8 1329.9 1335.9 1374.4 1419.1		
		H	0.6822	0.0031	1.8424	1451.0 1476.4 1503.0 1518.2 1557.1		

		C	0.6894	2.2443	0.0918	1607.7 1622.1 1630.9 2767.0 3148.3		
		C	-0.7123	2.1202	0.2402	3152.0 3157.3 3159.9 3168.5 3173.1		
		H	-1.3221	3.0221	0.2740	3181.3 3187.3 3190.9 3202.0		
		H	0.0741	2.4370	1.2414			
		C	-1.4221	0.8317	0.1078			
		C	-0.6893	-0.3571	0.2806			
		C	-2.7730	0.7802	-0.2499			
		C	-1.3266	-1.5777	0.0679			
		C	-3.4020	-0.4446	-0.4521			
		H	-3.3248	1.7058	-0.3813			
		C	-2.6739	-1.6222	-0.2962			
		H	-0.7771	-2.5043	0.1778			
		H	-4.4483	-0.4809	-0.7328			
		H	-3.1531	-2.5816	-0.4567			
		H	3.0121	1.7736	-1.0466			
TS49	-540.693364	C	-1.9619	-0.2566	0.1236	-2006.0 25.0 48.2 64.1 124.1 187.1	721.302	1
		C	-2.9632	-1.2218	0.2803	193.5 266.8 283.9 414.1 415.1 443.8	6864.991	
		C	-4.2972	-0.8976	0.0640	479.5 514.6 541.2 621.3 625.7 634.1	7402.879	
		C	-4.6494	0.4010	-0.3101	646.2 699.5 703.7 744.3 747.6 770.8		
		C	-3.6590	1.3649	-0.4707	790.3 827.5 834.7 858.0 883.6 896.6		
		C	-2.3188	1.0380	-0.2575	947.6 967.0 983.5 987.6 1003.0		
		H	-2.6893	-2.2259	0.5877	1003.2 1017.5 1046.8 1048.5 1068.5		
		H	-5.0632	-1.6547	0.1880	1099.3 1100.7 1169.9 1178.4 1182.0		
		H	-5.6903	0.6561	-0.4746	1185.5 1199.8 1206.1 1219.3 1252.8		
		H	-3.9239	2.3741	-0.7647	1306.0 1332.2 1347.2 1356.0 1358.5		
		H	-1.5482	1.7837	-0.4056	1364.3 1443.8 1478.3 1487.6 1524.8		
		C	-0.5120	-0.6343	0.2733	1526.0 1600.3 1622.8 1637.6 1641.8		
		H	-0.2050	-1.4752	-0.3420	2184.5 3127.7 3149.8 3154.0 3158.8		
		H	-0.6653	-1.6037	1.4811	3166.7 3167.3 3171.6 3177.6 3185.1		
		C	0.5147	0.3797	0.4489	3187.9 3188.8 3199.1		
		H	0.0161	-0.6585	1.4027			
		H	0.2126	1.3102	0.9118			
		C	1.9229	0.1670	0.1817			
		C	2.4607	-1.0543	-0.2811			
		C	2.8322	1.2296	0.3901			
		C	3.8231	-1.1927	-0.5343			
		H	1.8175	-1.9119	-0.4458			
		C	4.1876	1.0860	0.1319			
		H	2.4536	2.1800	0.7529			
		C	4.6990	-0.1281	-0.3345			
		H	4.2015	-2.1455	-0.8894			
		H	4.8536	1.9263	0.2973			
		H	5.7583	-0.2405	-0.5331			
TS50	-540.706035	C	1.9054	0.2177	-0.0099	-600.2 30.0 44.4 72.6 81.4 164.7	722.930	1
		C	2.7833	1.2514	0.3871	183.5 235.7 312.3 359.7 382.6 405.3	6874.869	
		C	4.1533	1.0488	0.4551	415.6 428.2 494.3 502.7 543.2 626.1	7313.827	
		C	4.6947	-0.1825	0.0740	634.7 637.6 685.9 703.4 714.9 760.6		
		C	3.8545	-1.2111	-0.3519	773.9 813.6 835.2 851.5 855.6 890.4		
		C	2.4765	-1.0235	-0.3696	925.6 942.2 982.8 989.8 998.0		
		H	2.3551	2.2144	0.6416	1005.4 1007.6 1013.3 1018.1 1038.2		
		H	4.8065	1.8516	0.7781	1047.0 1051.2 1100.5 1106.6 1150.9		
		H	5.7679	-0.3354	0.1015	1180.1 1182.8 1198.3 1199.9 1213.0		
		H	4.2753	-2.1627	-0.6574	1249.9 1306.3 1319.0 1345.2 1351.3		
		H	1.8397	-1.8402	-0.6875	1369.5 1423.4 1467.4 1484.5 1510.7		
		C	0.4865	0.5367	-0.1347	1524.3 1597.6 1623.5 1624.5 1642.3		
		H	-0.0128	1.2148	1.1763	2934.2 2976.9 3149.8 3159.7 3161.0		
		H	-0.1029	0.8764	1.9016	3169.7 3169.9 3179.2 3179.5 3186.7		
		C	-0.4605	-0.5913	-0.3767	3186.9 3191.4 3287.9		
		H	-0.2174	-1.5463	0.1113			
		H	-0.2920	-0.7692	-1.4559			
		C	-1.9313	-0.2782	-0.1802			
		C	-2.7609	-1.1880	0.4798			
		C	-2.4891	0.9091	-0.6665			
		C	-4.1191	-0.9213	0.6551			
		H	-2.3411	-2.1124	0.8649			

		C	-3.8448	1.1770	-0.4955			
		H	-1.8470	1.6252	-1.1667			
		C	-4.6655	0.2629	0.1665			
		H	-4.7464	-1.6371	1.1749			
		H	-4.2627	2.1017	-0.8786			
		H	-5.7208	0.4733	0.2999			
TS51	-539.494383	C	-1.9283	-0.2668	0.3374	-1938.8 29.7 49.1 52.2 143.5 152.0	782.855	3
		C	-3.0446	-1.1087	0.5099	240.4 275.7 284.5 408.9 415.4 460.2	6714.474	
		C	-4.2961	-0.7376	0.0360	486.5 507.9 536.1 613.2 625.6 632.9	6866.387	
		C	-4.4699	0.4871	-0.6141	680.2 685.4 703.3 756.2 779.8 814.5		
		C	-3.3728	1.3314	-0.7897	829.0 833.2 843.7 899.7 912.8 976.7		
		C	-2.1154	0.9617	-0.3244	978.1 983.1 987.6 992.6 1008.4		
		H	-2.9195	-2.0598	1.0178	1033.4 1040.8 1046.6 1094.5 1098.6		
		H	-5.1413	-1.4032	0.1732	1122.7 1174.7 1179.0 1189.7 1196.9		
		H	-5.4477	0.7771	-0.9808	1213.4 1277.7 1304.4 1337.4 1346.2		
		H	-3.4970	2.2811	-1.2987	1355.7 1454.2 1462.5 1481.2 1501.2		
		H	-1.2644	1.6171	-0.4734	1524.3 1568.8 1595.4 1602.0 1627.3		
		C	-0.6218	-0.6674	0.8586	2118.3 3070.5 3153.6 3158.7 3160.4		
		H	-0.4821	-1.7233	1.1003	3165.0 3170.4 3176.9 3177.2 3181.6		
		H	-0.1988	-0.0217	1.9087	3188.4 3190.4		
		C	0.5718	0.1473	0.8275			
		C	1.8930	0.0784	0.3540			
		C	2.9110	0.9448	0.8411			
		C	2.2523	-0.8721	-0.6466			
		C	4.2049	0.8596	0.3569			
		H	2.6534	1.6755	1.5992			
		C	3.5547	-0.9516	-1.1110			
		H	1.4893	-1.5348	-1.0391			
		C	4.5405	-0.0891	-0.6174			
		H	4.9659	1.5307	0.7400			
		H	3.8096	-1.6849	-1.8687			
		H	5.5570	-0.1549	-0.9871			
TS52	-539.473818	C	-1.9176	-0.5126	-0.2321	-2239.2 13.9 19.2 42.8 129.9 157.3	875.638	3
		C	-1.9363	0.8564	-0.5217	214.1 298.5 308.8 396.5 413.4 448.2	6353.585	
		C	-3.0863	1.6117	-0.3095	460.3 515.2 532.3 608.8 625.4 635.1	6460.982	
		C	-4.2371	1.0102	0.2014	685.3 710.2 741.4 747.2 786.9 811.3		
		C	-4.2270	-0.3504	0.4976	846.6 853.5 902.3 916.9 942.7 959.6		
		C	-3.0733	-1.1047	0.2816	971.1 973.2 981.6 998.9 1008.5		
		H	-1.0422	1.3332	-0.9097	1017.3 1043.4 1050.3 1100.7 1121.8		
		H	-3.0846	2.6713	-0.5406	1172.8 1180.9 1187.9 1202.7 1206.3		
		H	-5.1318	1.5990	0.3692	1243.4 1281.1 1312.9 1340.3 1360.3		
		H	-5.1147	-0.8269	0.8986	1408.0 1439.8 1447.1 1465.8 1482.6		
		H	-3.0726	-2.1645	0.5162	1524.8 1534.1 1606.7 1623.9 1641.6		
		C	-0.6669	-1.3435	-0.4856	1850.2 2971.6 3014.4 3154.1 3157.4		
		H	-0.4763	-1.3959	-1.5684	3158.9 3168.5 3170.0 3176.5 3181.4		
		H	-0.8567	-2.3744	-0.1611	3187.7 3188.7		
		C	0.5632	-0.8275	0.1644			
		C	1.8570	-0.3836	-0.1579			
		C	2.7177	-0.1711	-1.2572			
		C	2.3015	-0.0984	1.1484			
		C	3.9880	0.3225	-0.9660			
		H	2.4202	-0.3770	-2.2790			
		C	3.5481	0.3902	1.4527			
		H	0.9849	-0.5476	1.4920			
		C	4.4038	0.5996	0.3475			
		H	4.6850	0.5011	-1.7779			
		H	3.8749	0.6065	2.4626			
		H	5.4046	0.9823	0.5159			
TS53	-539.524656	C	1.5308	-0.7743	0.2324	-387.4 27.3 42.9 62.6 129.0 153.3	1355.998	1
		C	2.1939	0.0235	1.1678	232.0 315.4 322.1 407.2 412.0 425.6	4146.555	
		C	3.0627	1.0316	0.7571	488.1 528.9 585.1 635.0 654.3 665.3	4471.435	
		C	3.2812	1.2559	-0.6011	707.0 742.8 749.9 774.0 790.3 844.8		
		C	2.6296	0.4616	-1.5436	849.8 878.6 897.4 909.9 935.6 941.8		
		C	1.7655	-0.5483	-1.1276	977.4 986.4 996.3 1016.8 1021.6		
		H	2.0171	-0.1383	2.2258	1033.2 1051.6 1100.5 1121.2 1174.2		

		H	3.5658	1.6442	1.4971	1180.4 1194.4 1202.3 1211.5 1221.9		
		H	3.9572	2.0403	-0.9229	1280.1 1330.7 1338.4 1349.8 1361.1		
		H	2.7995	0.6243	-2.6023	1404.4 1453.5 1459.7 1481.8 1490.8		
		H	1.2654	-1.1649	-1.8680	1527.4 1571.1 1589.6 1624.1 1645.1		
		C	0.6252	-1.9006	0.6712	2950.9 3017.3 3072.1 3133.7 3147.6		
		H	0.9573	-2.8327	0.1838	3151.3 3153.1 3158.2 3167.6 3176.0		
		C	-0.8379	-1.7973	0.3549	3178.1 3186.7		
		C	-1.5906	-0.6863	-0.0880			
		C	-1.2060	0.3381	0.7592			
		C	-2.7832	-0.6547	-0.8591			
		C	-2.1199	1.3679	1.0172			
		C	-3.5129	0.5121	-0.8096			
		H	-3.1244	-1.5183	-1.4231			
		C	-3.1628	1.5351	0.1086			
		H	-1.9540	2.1053	1.7973			
		H	-4.3962	0.6379	-1.4260			
		H	-3.7329	2.4609	0.1006			
		H	0.7604	-2.0968	1.7413			
		H	-1.3686	-2.7475	0.4600			
TS54	-539.510025	C	-1.9944	-0.9517	0.3602	-551.7 18.5 59.2 86.3 141.3 222.8	1035.600	3
		C	-2.9861	-1.0486	-0.5802	265.4 313.4 371.0 408.6 424.8 450.7	4826.872	
		C	-3.7054	0.1092	-0.9587	486.2 534.4 574.7 604.3 624.2 682.4	5457.919	
		C	-3.3457	1.3584	-0.4418	695.7 719.9 739.7 751.2 798.7 821.9		
		C	-2.3407	1.4862	0.5108	824.7 873.1 889.6 913.5 947.4 968.9		
		C	-1.6328	0.3256	0.9503	972.1 979.9 983.2 997.7 1023.4		
		H	-3.1679	-1.9900	-1.0887	1025.8 1036.5 1064.9 1098.6 1110.2		
		H	-4.5014	0.0351	-1.6901	1163.9 1166.6 1174.0 1184.3 1190.6		
		H	-3.8851	2.2417	-0.7676	1227.1 1295.8 1307.6 1345.8 1347.8		
		H	-2.1221	2.4539	0.9480	1393.2 1441.7 1456.9 1461.4 1486.1		
		H	-1.2651	0.3375	1.9761	1495.0 1537.0 1566.1 1594.3 1612.4		
		C	-0.7320	-1.7720	0.5233	2964.1 3024.5 3081.3 3156.4 3157.5		
		H	-0.5557	-2.5075	-0.2702	3161.1 3164.0 3176.7 3177.1 3183.7		
		H	-0.6540	-2.2934	1.4893	3188.1 3190.8		
		C	0.0963	-0.5240	0.4609			
		C	1.4198	-0.1770	0.1737			
		C	2.3995	-1.1738	-0.1230			
		C	1.8439	1.1841	0.1614			
		C	3.7074	-0.8200	-0.4094			
		H	2.1091	-2.2183	-0.1211			
		C	3.1559	1.5177	-0.1245			
		H	1.1150	1.9565	0.3766			
		C	4.0998	0.5236	-0.4124			
		H	4.4341	-1.5943	-0.6317			
		H	3.4543	2.5605	-0.1276			
		H	5.1254	0.7923	-0.6365			
TS55	-539.429719	C	2.1072	1.0701	0.1458	-317.0 63.0 102.8 175.7 226.8 275.3	1074.505	1
		C	3.3378	0.5370	0.1085	323.9 358.2 397.3 442.2 474.2 483.0	3670.173	
		C	3.3946	-0.9453	0.2205	523.4 541.2 583.0 594.8 625.5 650.1	4587.496	
		C	2.3365	-1.7888	0.0129	689.4 706.9 722.9 749.4 798.0 816.8		
		C	1.0443	-1.1594	-0.3949	876.2 888.2 904.4 932.6 946.7 952.4		
		C	0.9934	0.0973	0.3184	969.3 975.0 977.5 979.6 990.0		
		H	4.2635	1.0891	-0.0177	1051.3 1061.0 1086.2 1130.6 1152.4		
		H	4.3725	-1.3871	0.3919	1163.3 1172.0 1186.3 1190.0 1198.4		
		H	2.5138	-2.8594	-0.0286	1220.7 1242.5 1292.1 1316.3 1332.5		
		H	0.9062	-0.1172	1.4033	1387.9 1400.8 1420.7 1444.4 1456.8		
		C	1.0780	2.2201	-0.0055	1514.1 1527.7 1612.4 1637.0 1682.8		
		H	1.1546	2.7942	-0.9330	2885.6 3029.0 3076.4 3077.4 3136.8		
		H	1.0269	2.9251	0.8308	3152.2 3154.3 3157.9 3164.6 3165.5		
		C	-0.0100	1.1006	-0.0412	3172.0 3182.9		
		C	-1.2249	0.5883	-0.3633			
		C	-2.5077	1.2506	-0.2365			
		C	-1.2360	-0.9166	-0.5139			
		C	-3.5756	0.5330	0.2008			
		H	-2.5595	2.3303	-0.3331			
		C	-2.3503	-1.5889	0.1155			

		H	-0.9944	-1.2965	-1.4977			
		C	-3.4635	-0.8837	0.4645			
		H	-4.5177	1.0295	0.4046			
		H	-2.3435	-2.6711	0.1936			
		H	-4.3220	-1.4041	0.8761			
		H	0.9565	-1.1193	-1.4797			
TS56	-539.437012	C	2.2737	0.8426	0.2206	-356.3 66.8 103.2 177.1 198.8 227.3	1143.740	1
		C	3.2040	-0.1269	-0.0517	300.5 356.2 392.1 417.2 456.8 493.9	3379.480	
		C	2.7997	-1.5362	-0.0397	507.0 525.3 532.5 570.7 609.8 631.6	4298.597	
		C	1.5039	-1.9135	-0.1968	689.6 694.4 731.5 751.6 764.9 775.6		
		C	0.5238	-0.7852	-0.4191	836.2 847.8 878.6 917.5 938.3 954.6		
		C	0.8903	0.3765	0.4750	964.3 969.6 977.9 985.5 1031.1		
		H	4.2461	0.1145	-0.2358	1053.8 1061.4 1115.6 1125.2 1152.0		
		H	3.5811	-2.2874	0.0014	1173.1 1187.6 1197.1 1204.7 1210.9		
		H	1.2470	-2.9580	-0.3405	1260.3 1282.3 1316.8 1349.5 1373.2		
		H	0.7426	0.1265	1.5386	1393.2 1403.6 1414.3 1431.3 1437.6		
		C	2.3206	2.2571	0.2809	1480.2 1545.6 1596.5 1605.8 1647.6		
		H	3.0415	2.8524	-0.2718	2903.5 2946.7 2953.6 3129.8 3149.9		
		H	1.7621	2.7621	1.0559	3153.9 3160.6 3162.2 3170.4 3178.0		
		C	-0.0756	1.4449	0.0262	3181.3 3236.9		
		C	-1.2213	0.8689	-0.3606			
		C	-2.6008	1.2915	-0.4816			
		C	-1.0229	-0.6965	-0.4677			
		C	-3.5598	0.4300	-0.0514			
		H	-2.8455	2.3061	-0.7774			
		C	-1.9755	-1.3759	0.4712			
		H	-1.3562	-0.9517	-1.4863			
		C	-3.2137	-0.8462	0.5714			
		H	-4.5999	0.7375	-0.0493			
		H	-1.7095	-2.2955	0.9825			
		H	-3.9766	-1.3467	1.1592			
		H	0.7893	-0.4453	-1.4373			
TS57	-539.426019	C	-2.5248	1.0090	-0.2088	-1224.5 63.2 74.4 137.6 205.7 233.4	1412.075	3
		C	-3.3683	-0.1379	-0.3174	257.0 369.2 392.9 422.2 437.9 446.0	2943.122	
		C	-2.7965	-1.4395	-0.4795	488.3 526.1 548.0 581.3 608.5 648.8	4102.994	
		C	-1.5255	-1.6980	-0.0527	664.2 676.7 697.9 733.4 748.1 769.6		
		C	-0.7895	-0.6353	0.7302	777.7 812.4 851.6 883.6 903.4 930.5		
		C	-1.1946	0.7303	0.1866	950.8 970.4 976.0 996.1 1014.7		
		H	-4.4435	-0.0083	-0.3763	1038.2 1083.8 1092.2 1107.5 1125.5		
		H	-3.3833	-2.2325	-0.9338	1140.2 1151.1 1169.6 1194.0 1224.7		
		H	-1.0915	-2.6856	-0.1594	1250.1 1265.1 1272.3 1298.7 1308.3		
		H	-1.5498	0.7904	-1.0510	1327.3 1377.5 1384.5 1404.1 1424.6		
		C	-0.0496	2.9736	0.0492	1425.9 1513.7 1530.7 1584.0 1608.1		
		H	0.8510	3.5753	0.0200	2154.3 2850.1 2936.9 3144.4 3146.9		
		H	-1.0055	3.4802	0.0086	3155.4 3159.2 3165.9 3174.3 3181.7		
		C	0.0022	1.6253	0.1424	3189.5 3238.6		
		C	1.1550	0.7508	0.1926			
		C	2.4327	0.9605	-0.3001			
		C	0.7747	-0.5994	0.7681			
		C	3.2939	-0.1225	-0.4931			
		H	2.7312	1.9474	-0.6392			
		C	1.5987	-1.7241	0.2124			
		H	1.0417	-0.5556	1.8431			
		C	2.8251	-1.4633	-0.3111			
		H	4.2840	0.0419	-0.9011			
		H	1.2571	-2.7457	0.3377			
		H	3.4605	-2.2828	-0.6303			
		H	-1.1543	-0.7019	1.7684			
TS58	-539.484946	C	2.5632	0.9529	-0.2685	-245.2 58.9 101.3 185.3 190.5 225.0	1197.760	1
		C	3.3377	-0.1063	0.1106	326.0 387.5 408.7 424.8 460.6 498.4	3074.074	
		C	2.7532	-1.3608	0.5546	518.6 540.6 580.3 605.3 642.2 677.1	3911.753	
		C	1.4551	-1.6561	0.3132	695.3 723.3 745.5 773.4 778.7 795.4		
		C	0.7198	-0.6929	-0.5633	803.9 864.9 915.8 924.5 951.7 964.3		
		C	1.1319	0.7653	-0.2898	968.2 974.6 974.7 989.6 1002.3		
		H	4.4100	0.0261	0.2007	1041.1 1076.2 1113.4 1137.8 1153.0		

		H	3.3775	-2.0441	1.1206	1176.4 1189.6 1195.9 1218.8 1224.8		
		H	0.9939	-2.5632	0.6853	1261.5 1294.2 1300.7 1310.5 1336.9		
		C	0.4349	2.1341	0.8181	1400.8 1407.2 1441.9 1460.2 1477.9		
		H	1.1942	2.9072	0.8298	1523.0 1565.1 1606.1 1632.6 1671.4		
		H	-0.0710	1.9302	1.7565	2909.6 2941.0 3113.2 3144.4 3156.4		
		C	-0.0630	1.5588	-0.3956	3158.3 3163.0 3166.4 3179.8 3184.5		
		C	-1.1968	0.8068	-0.5492	3188.6 3211.2		
		C	-2.4959	1.1470	-0.0376			
		C	-0.8331	-0.6558	-0.8392			
		C	-3.3345	0.1792	0.4115			
		H	-2.7710	2.1942	0.0357			
		C	-1.7377	-1.6089	-0.0960			
		H	-0.9580	-0.9069	-1.9044			
		C	-2.9054	-1.2129	0.4383			
		H	-4.3099	0.4355	0.8088			
		H	-1.4682	-2.6608	-0.1007			
		H	-3.5612	-1.9444	0.8995			
		H	1.1848	-0.8107	-1.5581			
		H	3.0023	1.9339	-0.4162			
TS59	-539.461099	C	-2.5676	1.0806	0.1446	-322.1 80.6 100.1 162.9 199.1 234.0	1097.204	1
		C	-3.4225	0.0136	0.2210	276.7 367.5 396.7 423.9 448.2 475.5	3277.809	
		C	-2.9684	-1.3383	-0.0698	524.4 559.6 576.8 587.9 633.9 687.2	4052.990	
		C	-1.6471	-1.6232	-0.0848	697.1 707.9 735.9 770.9 773.4 800.7		
		C	-0.7588	-0.5127	0.4105	844.2 924.6 930.3 950.7 968.3 970.2		
		C	-1.1878	0.8153	-0.1891	972.6 980.4 987.6 1000.9 1011.3		
		H	-4.4851	0.1923	0.3436	1069.8 1090.5 1149.8 1159.6 1165.6		
		H	-3.7077	-2.0909	-0.3228	1176.0 1188.0 1201.1 1207.5 1238.6		
		H	-1.2631	-2.6001	-0.3567	1271.1 1292.9 1329.8 1353.7 1362.3		
		C	-0.4634	1.7422	-1.0624	1390.7 1418.0 1429.5 1451.5 1485.9		
		H	-1.0287	2.6437	-1.2898	1514.4 1555.6 1586.0 1625.6 1656.7		
		H	0.0455	1.3695	-1.9509	2885.1 2917.4 3064.5 3125.2 3148.2		
		C	0.4609	1.8076	0.1236	3155.2 3158.1 3166.9 3173.3 3180.1		
		C	1.2740	0.7985	0.4873	3182.9 3198.3		
		C	2.7224	0.9639	0.5498			
		C	0.7605	-0.6319	0.5553			
		C	3.4936	-0.0222	0.0293			
		H	3.1407	1.9164	0.8496			
		C	1.5957	-1.5093	-0.3465			
		H	0.9488	-1.0394	1.5653			
		C	2.8991	-1.2312	-0.5301			
		H	4.5669	0.1141	-0.0478			
		H	1.1576	-2.4281	-0.7229			
		H	3.5326	-1.9094	-1.0911			
		H	-1.0931	-0.3797	1.4555			
		H	-2.9585	2.0940	0.1359			
TS60	-539.439865	C	-2.4638	0.8754	-0.7493	-1242.3 50.4 64.8 148.3 198.1 270.5	1361.506	3
		C	-3.2082	-0.3184	-0.7930	321.0 363.4 406.0 444.9 448.8 484.5	3023.113	
		C	-2.7605	-1.4537	-0.0678	501.8 521.8 557.0 581.2 627.3 653.5	3937.413	
		C	-1.6270	-1.4137	0.6867	669.2 689.2 728.6 746.3 778.3 785.4		
		C	-0.8092	-0.1638	0.8399	796.8 833.2 870.7 932.3 939.4 942.0		
		C	-1.2944	0.9684	-0.0339	967.9 977.3 1001.2 1008.7 1017.5		
		H	-4.1090	-0.3767	-1.3912	1057.5 1072.3 1121.8 1127.3 1142.4		
		H	-3.3375	-2.3713	-0.1167	1178.4 1195.3 1208.5 1214.8 1232.0		
		H	-1.3289	-2.2857	1.2588	1237.5 1282.2 1299.4 1307.6 1311.4		
		C	-0.4932	2.1920	0.0446	1331.3 1371.9 1395.6 1411.6 1417.1		
		H	0.0410	2.5341	1.1766	1441.9 1500.0 1533.3 1589.5 1598.0		
		H	-0.9884	3.1387	-0.1716	2028.1 2831.8 2852.3 3104.9 3148.7		
		C	0.9173	2.1929	0.2196	3154.3 3158.1 3171.8 3173.8 3184.5		
		C	1.4996	0.8784	0.3081	3191.8 3193.2		
		C	2.7694	0.7347	-0.2413			
		C	0.7590	-0.3695	0.7781			
		C	3.2742	-0.5106	-0.6327			
		H	3.3256	1.6397	-0.4585			
		C	1.2308	-1.6112	0.0582			
		H	1.0629	-0.5286	1.8330			

		C	2.4488	-1.6664	-0.5426			
		H	4.2549	-0.5799	-1.0881			
		H	0.6188	-2.5024	0.1258			
		H	2.7926	-2.5999	-0.9759			
		H	-0.9842	0.1885	1.8779			
		H	-2.8049	1.7361	-1.3178			
TS61	-539.482662	C	-2.3973	0.6009	-0.7283	-604.9 46.9 73.4 154.2 189.6 245.7	1545.454	3
		C	-2.7279	-0.6990	-1.1568	321.9 361.1 375.9 427.3 450.9 491.2	2835.321	
		C	-2.1665	-1.8111	-0.5007	510.1 513.2 578.3 594.4 609.1 670.7	3510.891	
		C	-1.3316	-1.6379	0.5758	709.2 721.2 733.5 740.7 794.4 823.4		
		C	-0.9331	-0.3131	1.0391	831.6 839.7 909.5 933.9 964.3 971.0		
		C	-1.5490	0.8116	0.3340	974.2 980.4 987.8 1020.8 1033.0		
		H	-3.3994	-0.8392	-1.9954	1036.6 1063.6 1118.2 1136.6 1145.2		
		H	-2.4204	-2.8129	-0.8304	1157.6 1168.5 1175.9 1193.3 1202.3		
		H	-0.9508	-2.5047	1.1049	1251.5 1266.1 1317.3 1334.2 1343.6		
		C	-0.9587	2.1867	0.6043	1401.8 1441.1 1454.2 1457.0 1460.3		
		H	-0.8849	2.3917	1.6854	1535.4 1537.8 1592.7 1595.9 1659.7		
		H	-1.5765	2.9773	0.1693	2940.7 3018.7 3060.2 3081.1 3145.0		
		C	0.3824	2.1245	-0.0265	3150.6 3158.1 3163.4 3171.9 3174.3		
		C	1.2351	1.0869	-0.0184	3187.4 3189.8		
		C	2.2908	0.8774	-0.9871			
		C	0.9456	0.0140	0.9976			
		C	2.9609	-0.2988	-1.0455			
		H	2.4960	1.6752	-1.6920			
		C	1.7444	-1.2101	0.8648			
		H	0.9752	0.4052	2.0129			
		C	2.6686	-1.3634	-0.1099			
		H	3.7260	-0.4547	-1.7973			
		H	1.5930	-1.9974	1.5972			
		H	3.2400	-2.2836	-0.1722			
		H	-0.9802	-0.2230	2.1278			
		H	-2.8005	1.4553	-1.2638			

Table S3: The energies (in kJ/mol) of the species and the transition states involved in the important reactions for phenanthrene formation from benzyl radicals (Figure 10) calculated at CBS-QB3, B3LYP/6-311++G(d,p) and M062X/6-311++G(d,p) levels of theory. The energies are relative to the energy of two benzyl radicals.

Species	***CBS-QB3***	***B3LYP/6-311++G(d,p)***	***M062X/6-311++G(d,p)***
Benzyl + benzyl	0	0	0
IS1	-283.2	-248.9	-305.5
IS2	-236.1	-221.1	-266.3
IS3	-350.2	-290.8	-350.0
IS4	-283.6	-201.9	-264.9
IS5	-350.6	-285.3	-320.7
IS7	-350.7	-324.5	-357.6
Phenanthrene	-242.4	-139.2	-179.3
TS3	-222.1	-186.5	-233.4
TS4	-241.3	-181.0	-239.1
TS5	-249.9	-193.2	-232.3
TS6	-226.2	-132.2	-163.1
TS10	-254.5	-233.6	-269.1
TS11	-76.1	-40.9	-73.2