

Supporting Information

Investigation of Polycyclic Aromatic Hydrocarbons (PAHs) Formation

Pathways in Butane or Butadiene Flames

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Table of Contents	Pages
Table S1 Barrier heights and reaction energies for steps involved in pyrene formation pathway from phenanthrene via C ₂ H ₃ addition computed at the G3(MP2, CC) level.	3
Table S2 Bibbs free energy barriers and reaction energies for steps involved in pyrene formation pathway from phenanthrene via C ₂ H ₃ addition computed at the G3(MP2, CC) level.	4
Table S3 Enthalpy barriers and reaction energies for steps involved in pyrene formation pathway from phenanthrene via C ₂ H ₃ addition computed at the G3(MP2, CC) level.	5
Table S4 Comparison of G3(MP2, CC) barrier heights for some steps optimized with B3LYP or CAM-B3LYP functionals.	6
Table S5 The molecular geometries (in Å), vibrational frequencies (in cm ⁻¹), moments of inertia (in amu) and zero-point vibrational energies (ZPE, in Hartree) of the chemical species (CS) and the transition states (TS) obtained at B3LYP/6-311++G(d, p).	7

Table S1 Barrier heights and reaction energies for steps involved in pyrene formation pathway

from phenanthrene via C₂H₃ addition computed at the G3(MP2, CC) level.

No.	Reaction	Barrier/ (kcal/mol)	Reaction heat/ (kcal/mol)
R1	2CS1=CS2	14.3	-119.7
R2	CS2+H=CS3+H ₂	22.4	13.1
Ra	CS2+O=CS3+OH	292.3	16.7
Rb	CS2+OH=CS3+H ₂ O	436.5	0.5
R3	CS3+C ₂ H ₃ =CS4	3.8	-116.2
R4	CS4+H=CS5+H ₂	23.6	13.0
R5	CS5=CS6	7.3	-39.7
R6	CS6=CS7+H	27.9	16.5
R7	CS8+C ₄ H ₄ =CS9	3.4	-48.1
R8	CS9=CS10	39.1	14.3
R9	CS10=CS11	38.6	2.4
R10	CS11=CS12	0.4	-65.1
R11	CS12=CS7+H	40.5	28.8
R13	CS13+C ₂ H ₃ =CS14	5.4	-113.0
R14	CS14+H=CS15+H ₂	31.0	11.9
R15	CS15=CS16	5.3	-53.2
R16	CS16=CS17+H	38.2	25.0
R17	CS18+C ₄ H ₄ =CS19	0.4	-51.0
R18	CS19=CS20	39.0	11.6
R19	CS20=CS21	7.9	-50.4
R20	CS21=CS22	37.3	0.7
R21	CS22=CS23	7.1	-38.7
R22	CS23=CS17+H	24.2	8.4
R23	CS24+C ₄ H ₄ =CS25	4.2	-48.2
R24	CS25=CS26	33.3	-47.4
R25	CS26=CS27		2.2
R26	CS27=CS28	40.7	13.6
R27	CS28=CS29	1.9	-73.8
R28	CS29=CS17+H	41.8	30.9

Table S2 Bibbs free energy barriers and reaction energies for steps involved in pyrene formation

pathway from phenanthrene via C₂H₃ addition computed at the G3(MP2, CC) level.

No.	Reaction	Barrier/ (kcal/mol)	Reaction heat/ (kcal/mol)
R1	2CS1=CS2	25.4	-101.9
R2	CS2+H=CS3+H ₂	26.8	10.0
Ra	CS2+O=CS3+OH	294.5	11.9
Rb	CS2+OH=CS3+H ₂ O	442.1	-0.7
R3	CS3+C ₂ H ₃ =CS4	15.1	-97.7
R4	CS4+H=CS5+H ₂	28.0	9.8
R5	CS5=CS6	8.2	-37.1
R6	CS6=CS7+H	23.9	5.6
R7	CS8+C ₄ H ₄ =CS9	14.2	-34.2
R8	CS9=CS10	37.1	15.3
R9	CS10=CS11	36.2	2.6
R10	CS11=CS12	0.7	-61.6
R11	CS12=CS7+H	35.8	17.3
R13	CS13+C ₂ H ₃ =CS14	16.5	-94.3
R14	CS14+H=CS15+H ₂	35.5	8.6
R15	CS15=CS16	5.7	-50.9
R16	CS16=CS17+H	33.8	17.8
R17	CS18+C ₄ H ₄ =CS19	9.6	-37.2
R18	CS19=CS20	37.0	12.7
R19	CS20=CS21	9.1	-46.9
R20	CS21=CS22	35.0	1.8
R21	CS22=CS23	7.5	-36.2
R22	CS23=CS17+H	20.2	-2.8
R23	CS24+C ₄ H ₄ =CS25	9.6	-34.1
R24	CS25=CS26	30.8	-47.4
R25	CS26=CS27	-	6.2
R26	CS27=CS28	38.2	14.7
R27	CS28=CS29	2.2	-70.8
R28	CS29=CS17+H	37.2	14.5

Table S3 Enthalpy barriers and reaction energies for steps involved in pyrene formation pathway from phenanthrene via C₂H₃ addition computed at the G3(MP2, CC) level.

No.	Reaction	Barrier/ (kcal/mol)	Reaction heat/ (kcal/mol)
R1	2CS1=CS2	14.4	-115.8
R2	CS2+H=CS3+H ₂	20.4	11.7
Ra	CS2+O=CS3+OH	287.5	14.3
Rb	CS2+OH=CS3+H ₂ O	443.8	0.6
R3	CS3+C ₂ H ₃ =CS4	4.4	-111.3
R4	CS4+H=CS5+H ₂	21.5	11.6
R5	CS5=CS6	6.4	-39.1
R6	CS6=CS7+H	23.4	12.0
R7	CS8+C ₄ H ₄ =CS9	3.1	-46.1
R8	CS9=CS10	36.1	15.1
R9	CS10=CS11	35.6	2.4
R10	CS11=CS12	-0.2	-64.4
R11	CS12=CS7+H	35.9	24.4
R13	CS13+C ₂ H ₃ =CS14	5.9	-108.1
R14	CS14+H=CS15+H ₂	28.8	10.4
R15	CS15=CS16	4.5	-52.5
R16	CS16=CS17+H	33.6	20.5
R17	CS18+C ₄ H ₄ =CS19	0.7	-49.1
R18	CS19=CS20	36.0	12.4
R19	CS20=CS21	7.0	-49.7
R20	CS21=CS22	33.7	1.1
R21	CS22=CS23	6.1	-38.0
R22	CS23=CS17+H	20.1	4.3
R23	CS24+C ₄ H ₄ =CS25	-0.5	-46.2
R24	CS25=CS26	29.7	-47.0
R25	CS26=CS27	-	3.4
R26	CS27=CS28	37.5	14.2
R27	CS28=CS29	0.8	-73.0
R28	CS29=CS17+H	37.2	26.3

Table S4 Comparison of G3(MP2, CC) barrier heights for some steps optimized with B3LYP or CAM-B3LYP functionals.

No.	Reaction	Barrier/ (kcal/mol) B3LYP	Barrier/ (kcal/mol) G3(MP2,CC) //B3LYP	Barrier/ (kcal/mol) cam-B3LYP	Barrier/ (kcal/mol) G3(MP2,CC) //CAM-B3LYP
R6	CS6=CS7+H	32.0	27.9	34.2	31.5
R7	CS8+C ₄ H ₄ =CS9	2.0	3.4	2.3	2.8
R10	CS11=CS12	2.8	0.4	1.4	2.4
R16	CS16=CS17+H	32.9	38.2	35.4	38.2
R18	CS19=CS20	38.7	39.0	40.3	33.2
R21	CS22=CS23	5.8	7.1	7.2	9.2
R22	CS23=CS17+H	18.3	24.2	20.6	19.2
R24	CS25=CS26	23.1	33.3	28.4	34.2

Table S5 The molecular geometries (in Å), vibrational frequencies (in cm⁻¹), moments of inertia (in amu) and zero-point vibrational energies (ZPE, in Hartree) of the chemical species (CS) and the transition states (TS) obtained at B3LYP/6-311++G(d, p).

Species	ZPE, Hartree	i	Ii	Cartesian coordinates, angstroms			vi, cm ⁻¹					
				Atom	X	Y	Z					
H ₂	0.010066	A	1811.1983	H	0	0	0.3000	4418				
				H	0	0	-0.3000					
C ₂ H ₂	0.026984	A	0.0000	C	0	0	0.6006	646	646	772	772	
				H	0	0	1.6706	2062	3420			
		C	50.7186	C	0	0	-0.6006					
				H	0	0	-1.6706					
C ₂ H ₃	0.036309	A	7.5985	C	0.0616	0.7587	0.0000	708	817	923	1041	
				H	-0.8661	1.2918	0.0000	1390	1645	3037	3135	
		C	62.9195	C	0.0616	-0.5965	0.0000	3238				
				H	-0.8629	-1.1352	0.0000					
				H	0.9893	-1.1297	0.0000					
C ₄ H ₄	0.060916	A	34.8795	C	-0.4546	1.8603	0.0000	226	321	558	653	
				H	-0.8651	2.8403	0.0000	686	703	891	956	
		C	416.6870	C	0.0000	0.7438	0.0000	1006	1110	1320	1442	
				C	0.5783	-0.5558	0.0000	1662	2199	3137	3147	
				H	1.6650	-0.5911	0.0000	3236			3476	
				C	-0.1204	-1.6971	0.0000					
				H	-1.2039	-1.7004	0.0000					
				H	0.3842	-2.6556	0.0000					
CS1	0.086921	A	286.7623	C	-1.2245	-0.7712	0.0000	3187	3176	3174	3161	
				C	0.0000	-1.3956	0.0000	3155	1626	1570	1467	
		C	608.07517	C	1.2245	-0.7712	0.0000	1460	1324	1301	1175	
				C	1.2124	0.6316	0.0000	1174	1071	1048	1014	
				C	0.0000	1.3225	0.0000	986	983	961	891	
				C	-1.2124	0.6316	0.0000	812	718	665	619	
				H	-2.1583	-1.3223	0.0000	600	424	398		
				H	2.1583	-1.3223	0.0000					
				H	2.1510	1.1761	0.0000					
				H	0.0000	2.4065	0.0000					
H	-2.1510	1.1761	0.0000									
CS2	0.180770	A	629.25887	C	-0.7428	0.0000	0.0000	65	93	125	267	
P2		B	3309.93836	C	-1.4638	1.1272	0.4216	312	367	413	419	
				C	-2.8563	1.1275	0.4218	502	556	625	628	
		C	3783.32350	C	-3.5591	0.0000	0.0000	639	710	713	753	
				C	-2.8563	-1.1275	-0.4218	755	795	855	855	
				C	-1.4638	-1.1272	-0.4216	922	939	984	984	
				C	0.7428	0.0000	0.0000	1001	1001	1010	1017	
				C	1.4638	1.1272	-0.4216	1025	1052	1066	1100	

				C	2.8563	1.1275	-0.4218	1105	1182	1182	1202
				C	3.5591	0.0000	0.0000	1209	1297	1301	1327
				C	2.8563	-1.1275	0.4218	1354	1358	1459	1487
				C	1.4638	-1.1272	0.4216	1514	1536	1607	1622
				H	-0.9284	2.0012	0.7748	1640	1642	3159	3160
				H	-3.3929	2.0069	0.7606	3165	3167	3174	3178
				H	-4.6432	0.0000	0.0000	3180	3183	3189	3191
				H	-3.3929	-2.0069	-0.7606				
				H	-0.9284	-2.0012	-0.7748				
				H	0.9284	2.0012	-0.7748				
				H	3.3929	2.0069	-0.7606				
				H	4.6432	0.0000	0.0000				
				H	3.3929	-2.0069	0.7606				
				H	0.9284	-2.0012	0.7748				
CS3	0.167635	A	608.90116	C	-0.7395	0.0027	0.0005	49	91	130	251
		B	3291.26432	C	-1.4852	-1.1235	-0.3017	314	381	413	419
		C	3822.68754	C	-2.8516	-1.2271	-0.3402	483	554	612	625
				C	-3.5805	-0.0701	-0.0262	639	693	705	741
				C	-2.9000	1.1026	0.3016	751	781	851	853
				C	-1.5071	1.1428	0.3180	929	943	982	984
				C	0.7432	0.0015	-0.0033	987	1000	1013	1024
				C	1.4472	-1.1788	0.2792	1048	1065	1100	1121
				C	2.8383	-1.1974	0.2805	1175	1182	1204	1239
				C	3.5566	-0.0359	-0.0017	1300	1319	1323	1356
				C	2.8695	1.1419	-0.2904	1432	1472	1481	1527
				C	1.4771	1.1603	-0.2934	1567	1614	1630	1641
				H	-3.3540	-2.1523	-0.6006	3158	3161	3165	3168
				H	-4.6649	-0.0936	-0.0358	3174	3177	3183	3187
				H	-3.4601	1.9955	0.5554	3191			
				H	-1.0025	2.0611	0.5987				
				H	0.8923	-2.0815	0.5090				
				H	3.3629	-2.1192	0.5067				
				H	4.6406	-0.0496	-0.0005				
				H	3.4182	2.0478	-0.5233				
				H	0.9588	2.0778	-0.5469				
CS4	0.213398	A	1472.69757	C	-0.9561	-0.2947	0.0345	43	81	88	109
		B	3566.13354	C	-1.5612	0.6486	0.8772	186	234	289	315
		C	4668.95155	C	-2.9444	0.8126	0.8874	325	416	427	474
				C	-3.7499	0.0389	0.0529	542	567	583	631
				C	-3.1617	-0.9025	-0.7898	635	666	715	733
				C	-1.7786	-1.0696	-0.7959	760	784	798	811
				C	0.5188	-0.5104	0.0432	859	890	935	937
				C	2.8161	0.2439	-0.1257	969	988	996	1004
				C	3.2777	-1.0396	0.1347	1013	1023	1031	1042

				C	2.3650	-2.0728	0.3425	1057	1079	1099	1126
				C	1.0021	-1.8033	0.2911	1181	1186	1203	1219
				H	-0.9432	1.2461	1.5374	1282	1292	1318	1323
				H	-3.3936	1.5418	1.5526	1340	1354	1449	1463
				H	-4.8263	0.1687	0.0597	1480	1506	1528	1597
				H	-3.7792	-1.5056	-1.4464	1614	1635	1640	1678
				H	-1.3264	-1.7966	-1.4616	3135	3154	3159	3162
				H	3.5288	1.0334	-0.3336	3166	3171	3176	3181
				H	4.3436	-1.2369	0.1587	3182	3190	3190	3218
				H	2.7116	-3.0804	0.5423				
				H	0.2896	-2.6010	0.4695				
				C	1.4435	0.5400	-0.1706				
				C	0.9887	1.9059	-0.4957				
				H	0.0160	1.9768	-0.9731				
				C	1.6583	3.0372	-0.2539				
				H	2.6144	3.0510	0.2587				
				H	1.2556	3.9968	-0.5556				
CS5	0.200103	A	1338.50498	C	-0.8151	-0.3351	0.0303	42	81	90	121
		B	3546.31403	C	-1.5988	-0.9803	-0.9044	192	212	272	298
		C	4390.93571	C	-2.9717	-1.0319	-0.9363	316	345	415	439
				C	-3.6485	-0.3750	0.1001	470	495	535	559
				C	-2.9201	0.2858	1.0915	607	622	631	682
				C	-1.5282	0.3090	1.0614	708	737	742	760
				C	0.6762	-0.3886	0.0010	765	832	858	870
				C	2.8956	0.5698	0.1038	947	958	965	984
				C	3.4694	-0.6951	0.1346	985	988	1011	1045
				C	2.6503	-1.8198	0.0789	1060	1090	1117	1131
				C	1.2700	-1.6575	0.0195	1174	1175	1220	1237
				H	-3.5130	-1.5540	-1.7178	1255	1309	1316	1318
				H	-4.7328	-0.3869	0.1307	1392	1430	1434	1455
				H	-3.4433	0.7851	1.8993	1468	1493	1559	1565
				H	-0.9754	0.8265	1.8380	1600	1625	3092	3117
				H	3.5353	1.4460	0.1273	3158	3161	3165	3170
				H	4.5465	-0.8007	0.1971	3175	3176	3178	3186
				H	3.0786	-2.8155	0.0987	3190			
				H	0.6249	-2.5288	0.0114				
				C	1.5057	0.7582	0.0088				
				C	1.0429	2.1562	-0.1213				
				H	1.7059	2.8850	0.3411				
				C	-0.0133	2.6188	-0.7951				
				H	-0.7077	1.9717	-1.3156				
				H	-0.2053	3.6845	-0.8475				
CS6	0.202383	A	1161.92643	C	-3.5803	-0.3363	-0.0001	31	90	170	221
		B	3315.31804	C	-2.8736	0.8461	-0.0001	249	276	396	426

			C	4466.38581	C	-1.4465	0.8610	-0.0001	432	448	495	498
					C	-0.7436	-0.3951	0.0000	548	563	630	672
					C	-1.4972	-1.5728	0.0001	696	713	717	729
					C	-2.8902	-1.5589	0.0001	761	782	818	850
					C	-0.7510	2.0730	-0.0001	863	864	927	940
					C	0.7341	-0.3920	0.0000	962	974	987	1007
					C	1.4445	0.8270	0.0001	1041	1060	1074	1113
					C	0.7330	2.1612	0.0002	1153	1175	1188	1197
					C	2.8430	0.8164	0.0000	1203	1217	1264	1297
					H	3.3740	1.7639	0.0000	1302	1330	1338	1375
					C	3.5600	-0.3725	-0.0001	1431	1447	1458	1483
					C	2.8666	-1.5839	-0.0001	1499	1533	1564	1603
					C	1.4802	-1.5877	-0.0001	1611	1642	2945	2947
					H	-1.3140	3.0008	-0.0002	3150	3157	3161	3168
					H	-4.6645	-0.3235	-0.0001	3172	3182	3185	3194
					H	-3.3969	1.7966	-0.0002	3207			
					H	-0.9993	-2.5338	0.0002				
					H	-3.4373	-2.4944	0.0002				
					H	1.0703	2.7503	-0.8681				
					H	4.6439	-0.3580	-0.0001				
					H	3.4074	-2.5236	-0.0001				
					H	0.9704	-2.5421	-0.0001				
					H	1.0700	2.7499	0.8689				
CS7	0.193561	A	1115.17950	C	3.5569	-0.2969	0.0000	95	100	227	242	
		B	3272.40099	C	2.8347	0.8773	-0.0001	248	400	411	436	
		C	4387.58048	C	1.4214	0.8653	0.0000	446	505	507	542	
				C	0.7283	-0.3792	0.0000	556	599	632	722	
				C	1.4979	-1.5646	0.0001	725	726	746	766	
				C	2.8783	-1.5281	0.0001	798	826	842	871	
				C	0.6786	2.0921	0.0000	879	887	955	966	
				C	-0.7283	-0.3792	0.0000	980	991	991	1016	
				C	-1.4214	0.8653	0.0000	1059	1060	1114	1164	
				C	-0.6786	2.0921	0.0000	1173	1185	1188	1224	
				C	-2.8347	0.8773	0.0000	1241	1266	1303	1324	
				H	-3.3464	1.8342	0.0001	1368	1374	1443	1449	
				C	-3.5569	-0.2969	0.0000	1469	1489	1533	1560	
				C	-2.8783	-1.5281	-0.0001	1606	1640	1652	1657	
				C	-1.4979	-1.5646	-0.0001	3155	3159	3160	3169	
				H	1.2288	3.0273	0.0000	3170	3175	3183	3186	
				H	4.6407	-0.2733	-0.0001	3193	3206			
				H	3.3464	1.8342	-0.0001					
				H	1.0055	-2.5284	0.0002					
				H	3.4406	-2.4551	0.0001					
				H	-1.2288	3.0273	0.0001					

				H	-4.6407	-0.2733	0.0000				
				H	-3.4406	-2.4551	-0.0001				
				H	-1.0055	-2.5284	-0.0001				
CS8	0.133723	A	573.07843	C	-2.3959	0.7952	0.0000	174	190	368	386
		B	1414.98779	C	-1.2358	1.4938	0.0000	471	486	510	520
		C	1988.06621	C	-0.0174	0.7449	0.0000	607	627	744	753
				C	-0.0869	-0.6867	0.0000	766	792	805	845
				C	-1.3560	-1.3274	0.0000	884	935	956	974
				C	-2.5256	-0.5934	0.0000	995	1038	1048	1140
				H	1.3050	2.4560	0.0000	1160	1172	1207	1249
				H	-1.2023	2.5785	0.0000	1276	1333	1384	1393
				C	1.2553	1.3722	0.0000	1455	1466	1527	1588
				C	1.1250	-1.4271	0.0000	1617	1652	3155	3159
				H	-1.3961	-2.4125	0.0000	3160	3164	3176	3180
				C	2.3429	-0.7903	0.0000	3188			
				C	2.4078	0.6227	0.0000				
				H	1.0741	-2.5110	0.0000				
				H	3.2594	-1.3693	0.0000				
				H	3.3742	1.1146	0.0000				
				H	-3.4944	-1.0797	0.0000				
CS9	0.198321	A	1126.38614	C	-0.8745	0.9515	-0.0716	31	49	102	150
		B	5029.65219	C	-0.2940	-0.3023	-0.1278	182	217	224	318
		C	6053.80906	C	1.1086	-0.4726	-0.0621	349	410	419	482
				C	1.9472	0.6811	0.0658	504	524	529	544
				C	1.3335	1.9588	0.1221	581	641	649	729
				C	-0.0310	2.0897	0.0559	750	754	776	779
				H	1.0833	-2.6314	-0.2151	809	842	874	908
				H	-0.9236	-1.1812	-0.2237	917	935	936	966
				C	1.7176	-1.7564	-0.1185	978	979	993	1039
				C	3.3538	0.5058	0.1317	1083	1147	1172	1176
				H	1.9611	2.8387	0.2190	1184	1190	1226	1263
				C	3.9104	-0.7496	0.0741	1288	1315	1383	1393
				C	3.0829	-1.8917	-0.0523	1402	1416	1469	1489
				H	3.9861	1.3825	0.2287	1498	1542	1604	1637
				H	4.9866	-0.8707	0.1252	1663	1884	3059	3096
				H	3.5338	-2.8768	-0.0968	3149	3156	3157	3161
				C	-2.3375	1.1582	-0.1389	3164	3174	3175	3187
				H	-2.6609	2.2005	-0.0779	3250			
				C	-3.2589	0.2378	-0.2598				
				C	-4.2242	-0.6941	-0.3953				
				H	-4.5089	-0.9564	-1.4150				
				C	-4.8815	-1.3447	0.6487				
				H	-4.6444	-1.1281	1.6825				
				H	-5.6456	-2.0821	0.4414				

				H	-0.4824	3.0754	0.1007				
CS10	0.199581	A	836.22404	C	-0.9095	0.4789	-0.0686	49	55	86	146
		B	5700.43574	C	-0.0424	-0.5785	-0.0281	178	193	211	303
		C	6505.05449	C	1.3494	-0.5437	0.0049	308	411	435	473
				C	1.9451	0.7691	-0.0072	497	516	522	580
				C	1.0878	1.9013	-0.0495	626	640	665	750
				C	-0.2775	1.7676	-0.0789	759	768	777	816
				H	1.7351	-2.6716	0.0600	867	891	924	934
				H	-2.5236	-1.7063	-0.2578	956	969	970	990
				C	2.1913	-1.6888	0.0501	991	1003	1027	1037
				C	3.3589	0.8693	0.0246	1081	1142	1167	1172
				H	1.5331	2.8904	-0.0579	1201	1235	1263	1313
				C	4.1459	-0.2575	0.0674	1330	1349	1360	1365
				C	3.5568	-1.5451	0.0808	1390	1444	1452	1490
				H	3.8122	1.8552	0.0145	1516	1574	1623	1644
				H	5.2257	-0.1638	0.0912	1663	1687	3123	3133
				H	4.1924	-2.4227	0.1153	3140	3144	3152	3158
				C	-2.3670	0.3750	-0.0985	3169	3175	3182	3192
				H	-2.9022	1.3211	-0.0798	3220			
				C	-3.0711	-0.7705	-0.1687				
				C	-4.5284	-0.8759	-0.1714				
				H	-4.9303	-1.7629	-0.6570				
				C	-5.3913	-0.0141	0.3826				
				H	-5.0588	0.8588	0.9343				
				H	-6.4612	-0.1697	0.3119				
				H	-0.9097	2.6499	-0.1102				
CS11	0.199755	A	1256.98257	C	1.1471	0.9793	0.0733	35	69	92	127
		B	3925.35874	C	0.4684	-0.2078	0.0620	180	188	244	322
		C	5150.97391	C	-0.9151	-0.3962	0.0225	384	418	427	467
				C	-1.7183	0.7974	-0.0182	500	519	524	594
				C	-1.0580	2.0569	-0.0093	623	666	697	748
				C	0.3086	2.1480	0.0336	761	772	783	800
				H	-0.9449	-2.5583	0.0415	831	871	895	931
				H	4.6030	0.7346	-0.1269	938	958	971	990
				C	-1.5568	-1.6643	0.0181	992	999	1021	1038
				C	-3.1284	0.6642	-0.0622	1089	1139	1161	1173
				H	-1.6590	2.9597	-0.0355	1194	1236	1262	1276
				C	-3.7199	-0.5779	-0.0626	1334	1352	1362	1398
				C	-2.9277	-1.7499	-0.0215	1439	1445	1471	1492
				H	-3.7374	1.5618	-0.0968	1515	1576	1617	1642
				H	-4.8001	-0.6638	-0.0968	1663	1676	3111	3123
				H	-3.4096	-2.7210	-0.0251	3139	3144	3151	3157
				C	2.5971	1.1675	0.1014	3169	3173	3181	3191
				H	2.8923	2.2068	0.2217	3224			

				C	3.6103	0.2913	-0.0806				
				C	3.5960	-1.1503	-0.3045				
				H	4.3756	-1.5077	-0.9760				
				C	2.7901	-2.0621	0.2558				
				H	2.0479	-1.7988	0.9987				
				H	2.8854	-3.1132	0.0069				
				H	0.7865	3.1231	0.0413				
CS12	0.202323	A	1151.03759	C	1.3721	0.9092	0.0000	84	116	164	221
		B	3303.34178	C	0.6949	-0.3216	0.0000	231	294	404	417
		C	4443.54346	C	-0.7319	-0.3484	0.0000	445	472	493	530
				C	-1.4641	0.8840	0.0000	539	542	604	653
				C	-0.7455	2.1143	0.0000	670	702	715	747
				C	0.6174	2.1254	0.0000	765	789	832	836
				H	-0.9542	-2.5097	0.0000	860	866	937	953
				H	4.6477	-0.1569	-0.0001	959	967	978	988
				C	-1.4760	-1.5612	0.0000	1003	1051	1071	1121
				C	-2.8777	0.8551	0.0000	1167	1174	1181	1200
				H	-1.3037	3.0448	0.0000	1204	1228	1235	1287
				C	-3.5654	-0.3386	0.0000	1314	1344	1382	1406
				C	-2.8532	-1.5560	0.0000	1415	1440	1444	1458
				H	-3.4166	1.7971	0.0000	1487	1542	1564	1588
				H	-4.6494	-0.3456	0.0000	1633	1645	2936	2940
				H	-3.3952	-2.4952	0.0000	3154	3155	3158	3168
				C	2.8009	0.9543	0.0000	3171	3174	3184	3184
				H	3.2925	1.9202	0.0000	3196			
				C	3.5649	-0.2274	0.0000				
				C	2.9669	-1.4559	0.0001				
				H	3.5671	-2.3594	0.0002				
				C	1.4786	-1.6170	0.0000				
				H	1.1816	-2.2295	0.8676				
				H	1.1816	-2.2295	-0.8676				
				H	1.1572	3.0666	0.0000				
CS13	0.180474	A	1093.99344	C	3.5598	-0.3684	0.0000	99	115	221	223
		B	3259.66075	C	2.8557	0.8188	0.0000	247	408	409	446
		C	4353.65419	C	1.4412	0.8411	0.0000	450	494	499	554
				C	0.7196	-0.3940	0.0000	556	586	628	705
				C	1.5076	-1.5413	0.0000	720	724	741	769
				C	2.8667	-1.6041	0.0000	794	826	835	880
				C	0.7007	2.0700	0.0000	887	888	965	968
				C	-0.7284	-0.3893	0.0000	983	995	1011	1049
				C	-1.4141	0.8555	0.0000	1064	1098	1162	1171
				C	-0.6586	2.0759	0.0000	1179	1189	1229	1242
				C	-2.8273	0.8611	0.0000	1281	1313	1354	1367
				H	-3.3469	1.8138	0.0000	1423	1430	1448	1474

				C	-3.5405	-0.3198	0.0000	1512	1531	1583	1633
				C	-2.8599	-1.5517	0.0000	1647	1652	3155	3159
				C	-1.4798	-1.5835	0.0000	3159	3166	3169	3174
				H	1.2535	3.0038	0.0000	3177	3182	3188	
				H	4.6445	-0.3634	0.0000				
				H	3.3892	1.7634	0.0000				
				H	3.4063	-2.5447	0.0000				
				H	-1.2004	3.0160	0.0000				
				H	-4.6245	-0.3011	0.0000				
				H	-3.4223	-2.4787	0.0000				
				H	-0.9541	-2.5319	0.0000				
CS14	0.226429	A	2122.34389	C	-3.6359	0.8337	0.0397	58	97	130	155
		B	3554.41093	C	-3.2415	-0.4781	-0.1145	226	240	276	312
		C	5616.70353	C	-1.8763	-0.8396	-0.0992	338	403	416	476
				C	-0.8705	0.1684	0.0230	500	509	514	541
				C	-1.3175	1.4940	0.2443	569	587	626	682
				C	-2.6606	1.8210	0.2474	703	727	742	758
				C	-1.5033	-2.2215	-0.1417	784	799	812	846
				C	0.5386	-0.2210	-0.0183	855	883	923	939
				C	0.8444	-1.6158	0.0489	969	979	985	988
				C	-0.2054	-2.5907	-0.0225	996	1011	1045	1055
				C	2.1813	-2.0538	0.1546	1071	1120	1153	1174
				H	2.3763	-3.1189	0.2203	1185	1196	1225	1241
				C	3.2192	-1.1494	0.1554	1254	1289	1319	1325
				C	2.9404	0.2111	-0.0140	1345	1362	1414	1441
				C	1.6374	0.6948	-0.1197	1451	1468	1480	1528
				H	-2.2865	-2.9672	-0.2278	1556	1602	1624	1645
				H	-4.6878	1.0959	0.0317	1659	1674	3130	3138
				H	-3.9823	-1.2627	-0.2289	3156	3159	3163	3170
				H	-0.6011	2.2724	0.4555	3176	3178	3185	3191
				H	-2.9588	2.8479	0.4269	3217	3230		
				H	0.0706	-3.6397	-0.0009				
				H	4.2466	-1.4861	0.2339				
				H	3.7596	0.9112	-0.1242				
				C	1.4827	2.1265	-0.4623				
				H	0.7597	2.3503	-1.2425				
				C	2.1899	3.1322	0.0601				
				H	2.8983	2.9786	0.8673				
				H	2.0675	4.1477	-0.2985				
CS15	0.212851	A	2106.73692	C	3.2744	-0.9885	0.0086	60	82	109	156
		B	3457.49098	C	2.2894	-1.9515	0.0522	225	231	246	301
		C	5520.62916	C	0.9269	-1.5861	0.0137	345	405	421	467
				C	0.5639	-0.2113	-0.0662	491	503	516	542
				C	1.5941	0.7733	-0.1430	565	575	624	675

				C	2.9235	0.3646	-0.0992	688	720	724	754
				C	-0.0952	-2.5929	0.0581	773	799	809	841
				C	-0.8462	0.1289	-0.0385	849	888	923	940
				C	-1.8393	-0.9041	0.0037	967	977	981	987
				C	-1.4142	-2.2717	0.0415	1005	1011	1054	1065
				C	-3.2090	-0.5546	0.0277	1107	1143	1172	1187
				H	-3.9449	-1.3511	0.0556	1192	1228	1250	1273
				C	-3.6210	0.7634	0.0250	1300	1321	1344	1355
				C	-2.6602	1.8013	0.0028	1407	1426	1443	1448
				C	-1.3510	1.4261	-0.0246	1471	1505	1523	1585
				H	0.2143	-3.6317	0.1054	1623	1641	1650	1666
				H	4.3205	-1.2723	0.0360	3128	3134	3156	3157
				H	2.5486	-3.0031	0.1147	3161	3167	3174	3176
				H	3.7014	1.1142	-0.1846	3180	3189	3218	
				H	-2.1715	-3.0482	0.0716				
				H	-4.6776	1.0085	0.0472				
				H	-2.9650	2.8421	0.0128				
				C	1.2930	2.2096	-0.3171				
				H	0.5734	2.4609	-1.0922				
				C	1.8693	3.1998	0.3715				
				H	2.5717	3.0041	1.1751				
				H	1.6381	4.2376	0.1614				
CS16	0.214991	A	1832.19022	C	3.5444	-0.0301	-0.0004	63	120	184	211
		B	3293.16172	C	2.8647	1.1818	-0.0003	238	288	352	402
		C	5114.48660	C	1.4465	1.2287	-0.0001	436	448	489	499
				C	0.7215	-0.0209	-0.0001	507	528	549	561
				C	1.4311	-1.2441	-0.0002	582	625	685	685
				C	2.8473	-1.2331	-0.0003	713	732	758	769
				C	0.7510	2.4377	-0.0001	793	802	816	836
				C	-0.7170	-0.0219	0.0001	871	899	937	947
				C	-1.4533	1.1910	0.0001	971	978	985	1002
				C	-0.7374	2.5258	0.0000	1048	1093	1109	1113
				C	-2.8381	1.1460	0.0003	1168	1188	1193	1197
				H	-3.4008	2.0748	0.0004	1210	1226	1256	1257
				C	-3.5273	-0.0770	0.0004	1319	1339	1362	1379
				C	-2.8264	-1.2661	0.0003	1415	1437	1439	1455
				C	-1.4165	-1.2649	0.0002	1459	1477	1522	1537
				C	-0.6646	-2.4848	0.0001	1584	1602	1636	1649
				C	0.6950	-2.4754	-0.0001	2952	2953	3152	3155
				H	1.2498	-3.4079	-0.0001	3157	3161	3163	3170
				H	-1.2069	-3.4247	0.0001	3174	3183	3184	
				H	1.3112	3.3672	-0.0001				
				H	4.6289	-0.0366	-0.0005				
				H	3.4166	2.1157	-0.0003				

				H	3.3819	-2.1767	-0.0004				
				H	-1.0711	3.1154	0.8688				
				H	-4.6116	-0.0828	0.0005				
				H	-3.3527	-2.2148	0.0004				
				H	-1.0712	3.1154	-0.8687				
CS17	0.206163	A	1782.55145	C	3.5194	0.0000	0.0003	97	150	210	246
		B	3244.15401	C	2.8296	-1.2091	0.0003	260	358	402	411
		C	5026.70546	C	1.4273	-1.2343	0.0002	462	499	505	507
				C	0.7128	0.0000	0.0001	507	538	553	581
				C	1.4273	1.2343	0.0001	594	687	703	718
				C	2.8296	1.2091	0.0003	748	752	766	809
				C	0.6795	-2.4612	0.0001	811	814	833	854
				C	-0.7128	0.0000	-0.0001	902	916	974	979
				C	-1.4273	-1.2343	-0.0001	980	982	989	1014
				C	-0.6795	-2.4612	0.0000	1089	1112	1125	1164
				C	-2.8296	-1.2091	-0.0003	1166	1197	1203	1230
				H	-3.3758	-2.1460	-0.0003	1261	1262	1266	1342
				C	-3.5194	0.0000	-0.0004	1350	1399	1425	1432
				C	-2.8296	1.2091	-0.0003	1456	1458	1481	1512
				C	-1.4273	1.2343	-0.0002	1532	1592	1624	1632
				C	-0.6795	2.4612	-0.0001	1642	1667	3161	3161
				C	0.6795	2.4612	0.0001	3164	3164	3170	3172
				H	1.2271	3.3974	0.0002	3180	3180	3188	3189
				H	-1.2271	3.3974	-0.0001				
				H	1.2271	-3.3974	0.0002				
				H	4.6031	0.0000	0.0004				
				H	3.3758	-2.1460	0.0003				
				H	3.3758	2.1460	0.0004				
				H	-1.2271	-3.3974	0.0000				
				H	-4.6031	0.0000	-0.0005				
				H	-3.3758	2.1460	-0.0004				
CS18	0.142704	A	1175.87563	C	-1.7281	-1.9791	0.0001	103	138	176	207
		B	1892.59436	C	-0.4048	-1.6894	-0.0001	356	363	436	445
		C	3068.46999	C	-0.0351	-0.3105	0.0000	479	490	551	568
				C	-1.0702	0.6798	0.0002	587	632	644	696
				C	-2.4325	0.2728	0.0003	701	744	768	791
				C	-2.7785	-1.0634	0.0002	827	862	868	928
				H	0.3656	-2.4521	-0.0002	960	987	1029	1053
				C	1.3350	0.1175	-0.0002	1094	1150	1191	1215
				C	-0.7142	2.0534	0.0002	1241	1277	1325	1355
				H	-3.2054	1.0352	0.0004	1386	1446	1471	1512
				H	-3.8163	-1.3768	0.0003	1592	1612	1636	2195
				C	0.6050	2.4394	0.0001	3157	3165	3177	3180
				C	1.6291	1.4730	-0.0001	3180	3194	3475	

				H	-1.5037	2.7974	0.0004				
				H	0.8668	3.4912	0.0001				
				H	2.6664	1.7852	-0.0002				
				C	2.3933	-0.8388	-0.0003				
				C	3.2911	-1.6432	-0.0005				
				H	4.0860	-2.3483	-0.0006				
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CS19	0.207231	A	2107.56530	C	-0.9778	-1.3211	-0.0987	24	45	86	115
		B	5081.48293	C	-0.3546	-0.0853	-0.1017	127	158	187	222
		C	7076.44421	C	1.0507	0.0338	-0.0244	230	312	340	386
				C	1.8465	-1.1533	0.0592	403	448	454	508
				C	1.1887	-2.4103	0.0606	517	528	551	580
				C	-0.1781	-2.4928	-0.0158	586	593	636	672
				H	-0.9517	0.8168	-0.1637	695	712	734	751
				C	1.7175	1.3087	-0.0262	758	785	819	854
				C	3.2578	-1.0473	0.1381	872	912	925	927
				H	1.7877	-3.3128	0.1237	935	953	973	985
				H	-0.6634	-3.4632	-0.0133	1047	1082	1094	1175
				C	3.8704	0.1834	0.1348	1179	1190	1199	1231
				C	3.1005	1.3608	0.0525	1253	1289	1308	1351
				H	3.8479	-1.9555	0.2015	1389	1402	1419	1472
				H	4.9500	0.2577	0.1951	1476	1489	1537	1603
				H	3.5907	2.3267	0.0501	1626	1653	1883	2194
				C	0.9691	2.5200	-0.1085	3059	3098	3149	3158
				C	0.3427	3.5477	-0.1778	3163	3175	3180	3184
				H	-0.2071	4.4550	-0.2380	3194	3251	3475	
				C	-2.4465	-1.4718	-0.1788				
				H	-2.8069	-2.5036	-0.1700				
				C	-3.3335	-0.5134	-0.2549				
				C	-4.2653	0.4569	-0.3450				
				H	-4.5349	0.7808	-1.3509				
				C	-4.9038	1.0757	0.7293				
				H	-4.6778	0.7994	1.7512				
				H	-5.6398	1.8500	0.5580				
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CS20	0.208491	A	1952.88612	C	1.0036	-1.1075	0.0000	33	61	83	112
		B	5729.80452	C	0.2011	0.0019	0.0000	122	156	183	215
		C	7682.69064	C	-1.1883	0.0486	0.0000	244	290	319	372
				C	-1.8628	-1.2232	0.0000	381	452	469	491
				C	-1.0743	-2.4055	0.0000	520	535	554	580
				C	0.2967	-2.3557	0.0000	589	632	644	684
				C	-1.9619	1.2574	0.0000	694	712	747	756
				C	-3.2788	-1.2446	0.0000	781	831	870	895
				H	-1.5796	-3.3652	0.0000	924	928	959	960
				H	0.8742	-3.2752	0.0000	965	975	983	1038
				C	-4.0002	-0.0725	0.0000	1041	1088	1158	1171

				C	-3.3450	1.1757	0.0000	1191	1221	1244	1259
				H	-3.7879	-2.2027	0.0000	1293	1314	1324	1345
				H	-5.0836	-0.1012	0.0000	1358	1394	1443	1455
				H	-3.9257	2.0900	0.0000	1468	1510	1577	1621
				C	-1.3069	2.5230	0.0000	1628	1651	1687	2197
				C	-0.7596	3.5969	0.0000	3125	3132	3136	3141
				H	-0.2759	4.5428	-0.0001	3153	3163	3176	3181
				C	2.4630	-1.0866	-0.0001	3195	3223	3476	
				H	2.9472	-2.0607	-0.0001				
				C	3.2339	0.0197	0.0000				
				C	4.6813	-0.0057	0.0000				
				H	5.1505	-0.9878	-0.0002				
				C	5.4575	1.0883	0.0001				
				H	5.0297	2.0857	0.0002				
				H	6.5383	1.0173	0.0000				
				H	2.7558	0.9970	0.0002				
CS21	0.211293	A	2133.63287	C	3.6769	0.3905	0.0001	37	102	134	164
		B	3475.10892	C	3.0820	-0.8837	0.0000	185	220	238	295
		C	5598.06311	C	1.6636	-1.0452	0.0000	364	381	412	470
				C	0.7977	0.0695	0.0000	496	499	502	531
				C	1.4090	1.4575	0.0001	544	586	593	621
				C	2.9038	1.5135	0.0001	649	666	681	685
				C	1.1263	-2.3685	0.0000	718	755	770	789
				C	-0.6228	-0.1286	0.0000	807	840	844	930
				C	-1.1257	-1.4797	0.0000	932	934	968	976
				C	-0.2158	-2.5756	-0.0001	983	993	1003	1090
				C	-2.5113	-1.7439	-0.0001	1118	1151	1179	1184
				H	-2.8384	-2.7783	-0.0001	1199	1218	1219	1246
				C	-3.4308	-0.7205	-0.0001	1265	1307	1337	1345
				C	-2.9762	0.6025	0.0000	1387	1415	1425	1440
				C	-1.6183	0.9229	0.0000	1455	1475	1532	1570
				H	1.8148	-3.2069	0.0000	1583	1620	1644	2179
				H	4.7587	0.4739	0.0001	2984	2987	3155	3159
				H	3.7011	-1.7733	0.0000	3164	3171	3178	3181
				H	1.0330	2.0266	-0.8612	3184	3196	3473	
				H	3.3595	2.4979	0.0001				
				H	-0.6211	-3.5818	-0.0001				
				H	-4.4945	-0.9271	-0.0001				
				H	-3.6906	1.4164	0.0000				
				H	1.0330	2.0266	0.8613				
				C	-1.3533	2.3286	0.0000				
				C	-1.2835	3.5332	0.0000				
				H	-1.1850	4.5910	0.0001				
CS22	0.212430	A	2081.82819	C	3.6380	0.7403	-0.0463	58	98	127	156

		B	3532.86060	C	3.1992	-0.5530	0.1419	224	239	279	319
		C	5553.36521	C	1.8233	-0.8701	0.1227	343	403	416	479
				C	0.8535	0.1674	-0.0343	507	510	516	539
				C	1.3450	1.4700	-0.2938	568	583	615	668
				C	2.6983	1.7525	-0.2946	678	725	733	756
				C	1.4027	-2.2377	0.1899	782	789	802	837
				C	-0.5677	-0.1741	0.0040	847	860	881	889
				C	-0.9209	-1.5584	-0.0480	927	971	980	988
				C	0.0951	-2.5661	0.0564	997	1002	1012	1068
				C	-2.2704	-1.9496	-0.1685	1113	1150	1174	1184
				H	-2.5027	-3.0078	-0.2236	1193	1221	1240	1241
				C	-3.2760	-1.0082	-0.1996	1264	1292	1322	1344
				C	-2.9535	0.3425	-0.0376	1362	1416	1446	1464
				C	-1.6354	0.7756	0.0896	1479	1527	1556	1601
				H	2.1591	-3.0072	0.3024	1622	1640	1648	1658
				H	4.6979	0.9678	-0.0360	3029	3157	3159	3163
				H	3.9130	-1.3578	0.2846	3170	3176	3178	3186
				H	0.6562	2.2631	-0.5407	3190	3227	3245	
				H	3.0324	2.7622	-0.5052				
				H	-0.2154	-3.6055	0.0494				
				H	-4.3127	-1.3096	-0.2964				
				H	-3.7438	1.0794	0.0425				
				C	-1.4311	2.2030	0.4402				
				C	-2.1418	3.2201	0.0078				
				H	-2.1890	4.2865	0.1682				
				H	-0.6452	2.4048	1.1755				
CS23	0.214547	A	1822.34400	C	-3.5354	-0.0585	-0.0604	81	133	193	216
		B	3283.97187	C	-2.8884	1.1599	-0.0209	244	337	382	396
		C	5062.75504	C	-1.4770	1.2260	0.0261	442	457	487	498
				C	-0.7271	0.0093	0.0699	506	521	538	550
				C	-1.4143	-1.2467	-0.0157	580	650	673	679
				C	-2.7985	-1.2584	-0.0765	705	732	761	774
				C	-0.7663	2.4617	0.0189	798	811	818	844
				C	0.6829	0.0532	0.1396	849	911	946	959
				C	1.3653	1.2792	0.0476	971	978	987	990
				C	0.5998	2.4867	0.0061	1061	1073	1093	1098
				C	2.7860	1.2850	-0.0755	1141	1168	1173	1188
				H	3.3029	2.2342	-0.1595	1198	1216	1231	1255
				C	3.4996	0.0778	-0.2305	1260	1294	1334	1371
				C	2.8875	-1.1367	-0.0862	1397	1413	1418	1425
				C	1.4653	-1.2173	0.3959	1457	1476	1520	1553
				C	0.7117	-2.4634	0.0090	1584	1621	1628	1681
				C	-0.6214	-2.4653	-0.1264	2750	3148	3155	3156
				H	-1.1473	-3.3887	-0.3492	3158	3165	3169	3172

				H	1.2811	-3.3824	-0.0896	3174	3182	3184	
				H	-1.3311	3.3880	-0.0015				
				H	-4.6182	-0.0962	-0.0999				
				H	-3.4577	2.0833	-0.0364				
				H	-3.3199	-2.2070	-0.1527				
				H	1.1279	3.4335	-0.0413				
				H	4.5527	0.1203	-0.4894				
				H	3.4390	-2.0617	-0.2153				
				H	1.5525	-1.2786	1.5089				
CS24	0.142679	A	1201.89511	C	-1.8608	-1.9119	0.0000	105	126	169	201
		B	1898.15438	C	-0.5478	-1.5764	-0.0001	339	364	443	453
		C	3100.04949	C	-0.0186	-0.2824	0.0000	476	489	542	577
				C	-0.9813	0.7855	0.0002	592	626	647	694
				C	-2.3661	0.4633	0.0003	702	749	757	798
				C	-2.7999	-0.8411	0.0002	812	867	883	926
				C	1.3807	0.0241	-0.0001	970	988	1020	1051
				C	-0.5109	2.1235	0.0002	1087	1164	1188	1196
				H	-3.0856	1.2749	0.0004	1238	1262	1343	1358
				H	-3.8612	-1.0657	0.0003	1398	1452	1464	1506
				C	0.8373	2.3952	0.0001	1583	1621	1651	2199
				C	1.7832	1.3503	-0.0001	3159	3163	3170	3180
				H	-1.2344	2.9321	0.0004	3182	3195	3477	
				H	1.1844	3.4222	0.0001				
				H	2.8418	1.5796	-0.0002				
				C	2.3409	-1.0298	-0.0003				
				C	3.1568	-1.9166	-0.0005				
				H	3.8719	-2.7024	-0.0006				
				H	-2.1981	-2.9425	0.0000				
CS25	0.207298	A	2085.42594	C	0.8473	-1.8113	-0.0899	27	44	62	130
		B	4609.11605	C	0.5026	-0.4706	-0.1623	153	172	185	196
		C	6620.10735	C	-0.8830	-0.0939	-0.0679	235	325	344	369
				C	-1.8576	-1.1489	0.0311	392	475	479	502
				C	-1.4424	-2.5034	0.0931	515	527	547	564
				C	-0.1113	-2.8286	0.0526	586	614	635	650
				C	-1.3825	1.2604	-0.0419	686	701	744	767
				C	-3.2429	-0.8477	0.0764	775	798	811	812
				H	-2.2010	-3.2744	0.1717	844	905	922	933
				H	0.2067	-3.8638	0.1014	938	985	991	1000
				C	-3.6863	0.4494	0.0473	1046	1092	1115	1139
				C	-2.7528	1.4965	0.0010	1185	1189	1193	1230
				H	-3.9470	-1.6706	0.1389	1244	1279	1298	1351
				H	-4.7459	0.6747	0.0789	1369	1386	1420	1458
				H	-3.0953	2.5238	0.0167	1483	1490	1540	1604
				C	-0.5648	2.4333	-0.0036	1627	1641	1889	2188

				C	0.0098	3.4918	0.0568	3098	3122	3148	3163
				H	0.5512	4.4045	0.1098	3166	3177	3182	3189
				H	1.8943	-2.0768	-0.1772	3196	3249	3474	
				C	1.5920	0.5120	-0.3933				
				H	1.3467	1.3852	-0.9924				
				C	2.8185	0.3913	0.0409				
				C	4.0870	0.3268	0.4950				
				H	4.2842	0.8055	1.4548				
				C	5.1560	-0.2953	-0.1503				
				H	5.0273	-0.7839	-1.1079				
				H	6.1418	-0.2952	0.2954				
CS26	0.207871	A	2164.88647	C	-0.1860	-2.3285	0.0806	31	40	52	100
		B	4570.65370	C	-0.3087	-0.9406	0.0715	122	161	193	198
		C	6706.54911	C	0.8771	-0.1147	0.0574	249	287	326	348
				C	2.1441	-0.7902	-0.0339	402	436	473	488
				C	2.2057	-2.2072	-0.0303	508	538	549	567
				C	1.0638	-2.9644	0.0421	601	637	650	673
				C	0.8866	1.3221	0.1078	693	759	770	774
				C	3.3457	-0.0437	-0.1356	801	822	843	864
				H	3.1796	-2.6811	-0.0896	901	921	937	938
				H	1.1164	-4.0469	0.0491	984	991	1000	1018
				C	3.3197	1.3271	-0.1381	1052	1102	1116	1155
				C	2.0929	1.9979	-0.0002	1189	1201	1228	1253
				H	4.2846	-0.5816	-0.2089	1271	1304	1317	1349
				H	4.2384	1.8971	-0.2170	1371	1393	1446	1459
				H	2.0785	3.0796	0.0584	1483	1538	1600	1624
				C	-0.3313	2.1335	0.3393	1634	1646	1656	2280
				C	-0.5505	3.3391	-0.1360	3074	3124	3146	3162
				H	-1.3232	4.0901	-0.0717	3166	3178	3181	3190
				H	-1.0917	-2.9222	0.0962	3195	3236	3243	
				C	-1.6402	-0.4393	0.0190				
				C	-2.8140	-0.1446	-0.0576				
				C	-4.1548	0.2985	-0.1584				
				H	-4.2884	1.3653	-0.3277				
				C	-5.2365	-0.4893	-0.0650				
				H	-5.1505	-1.5565	0.1013				
				H	-6.2330	-0.0747	-0.1551				
				H	-1.0926	1.6981	0.9885				
CS27	0.211349	A	1696.79457	C	0.7034	1.7796	-0.1106	38	56	126	154
		B	4569.26463	C	0.4093	0.4237	-0.0924	180	216	226	319
		C	6164.12146	C	-0.9550	0.0123	-0.0170	346	357	441	474
				C	-1.9896	0.9973	0.0312	479	495	502	510
				C	-1.6371	2.3678	0.0062	535	563	575	610
				C	-0.3142	2.7463	-0.0621	646	680	702	751

				C	-1.3090	-1.3746	0.0123	759	775	797	807
				C	-3.3455	0.5724	0.1038	826	834	907	908
				H	-2.4232	3.1144	0.0430	915	927	981	988
				H	-0.0497	3.7977	-0.0787	992	1013	1055	1097
				C	-3.6620	-0.7642	0.1291	1118	1134	1152	1179
				C	-2.6438	-1.7387	0.0841	1187	1202	1222	1240
				H	-4.1265	1.3244	0.1393	1260	1298	1362	1382
				H	-4.6986	-1.0771	0.1848	1391	1419	1428	1465
				H	-2.9065	-2.7912	0.1068	1486	1492	1537	1611
				C	-0.2472	-2.3636	-0.0322	1621	1630	1668	1842
				C	1.0510	-2.0167	-0.1059	3074	3148	3158	3160
				H	1.8263	-2.7728	-0.1388	3161	3167	3173	3184
				H	1.7388	2.0971	-0.1624	3185	3188	3250	
				C	1.4767	-0.6141	-0.1514				
				H	-0.5276	-3.4116	-0.0043				
				C	2.7624	-0.3167	-0.2475				
				C	4.0704	-0.0254	-0.3720				
				H	4.4583	0.0646	-1.3892				
				C	4.9713	0.1730	0.6770				
				H	4.6550	0.0989	1.7097				
				H	6.0080	0.4060	0.4727				
CS28	0.212432	A	1698.20085	C	0.0725	2.1273	-0.0473	50	77	136	165
		B	4422.81799	C	0.2597	0.7692	-0.0787	176	211	238	266
		C	6068.29012	C	-0.9480	-0.0070	-0.0252	348	389	446	457
				C	-2.2194	0.6424	0.0584	468	485	502	528
				C	-2.2839	2.0575	0.0852	537	595	613	646
				C	-1.1239	2.8149	0.0315	676	693	755	762
				C	-0.8858	-1.4344	-0.0560	773	787	807	827
				C	-3.3943	-0.1585	0.1151	837	891	907	912
				H	-3.2519	2.5442	0.1477	933	945	982	998
				H	-1.1607	3.8985	0.0503	1012	1031	1054	1095
				C	-3.3136	-1.5307	0.0868	1108	1132	1143	1183
				C	-2.0610	-2.1696	-0.0007	1202	1226	1257	1284
				H	-4.3584	0.3338	0.1821	1320	1332	1368	1376
				H	-4.2167	-2.1288	0.1305	1395	1429	1456	1462
				H	-2.0104	-3.2531	-0.0273	1480	1511	1572	1580
				C	0.4148	-2.0612	-0.1724	1614	1627	1650	1665
				C	1.5607	-1.3464	-0.2047	3109	3129	3143	3158
				H	2.5051	-1.8590	-0.3261	3160	3162	3169	3176
				C	1.5773	0.1030	-0.1315	3185	3208	3227	
				H	0.4494	-3.1429	-0.2534				
				C	2.7232	0.8503	-0.1498				
				C	4.1115	0.4228	-0.1246				
				H	4.7936	1.0937	-0.6456				

				C	4.6549	-0.6291	0.5100				
				H	4.0731	-1.3027	1.1275				
				H	5.7214	-0.8140	0.4573				
				H	2.5875	1.9274	-0.2196				
CS29	0.215186	A	1790.74654	C	3.5684	-0.0370	-0.0004	86	98	183	205
		B	3350.31294	C	2.8914	1.1818	-0.0003	254	321	347	403
		C	5130.19078	C	1.4822	1.2266	-0.0002	431	452	486	493
				C	0.7499	-0.0031	-0.0001	505	513	541	541
				C	1.4525	-1.2455	-0.0001	590	655	660	683
				C	2.8692	-1.2355	-0.0003	732	736	749	786
				C	0.7580	2.4514	-0.0001	800	809	828	837
				C	-0.6775	0.0117	0.0001	884	936	943	952
				C	-1.3674	1.2703	0.0001	966	970	976	987
				C	-0.6237	2.4606	0.0000	998	1096	1134	1144
				C	-2.8135	1.2747	0.0003	1168	1191	1202	1209
				H	-3.3153	2.2377	0.0003	1215	1224	1242	1262
				C	-3.5363	0.1404	0.0004	1317	1338	1367	1380
				C	-2.9053	-1.2194	0.0003	1407	1431	1447	1448
				C	-1.3933	-1.2084	0.0002	1457	1493	1524	1545
				C	-0.6823	-2.4170	0.0001	1583	1594	1602	1660
				C	0.6993	-2.4468	0.0000	2960	2961	3147	3149
				H	1.2235	-3.3965	-0.0001	3155	3159	3168	3169
				H	-1.2348	-3.3521	0.0002	3173	3175	3183	
				H	1.3095	3.3853	-0.0002				
				H	4.6528	-0.0472	-0.0005				
				H	3.4477	2.1130	-0.0004				
				H	3.4021	-2.1803	-0.0003				
				H	-1.1546	3.4073	0.0001				
				H	-4.6207	0.1850	0.0005				
				H	-3.2695	-1.7896	0.8693				
				H	-3.2697	-1.7896	-0.8685				
TS1	0.173804	A	834.13395	C	1.2285	0.8262	0.8253	-423	25	47	76
		B	3222.61892	C	1.7694	-0.3418	1.3747	139	153	309	389
		C	3499.69995	C	2.5906	-1.1016	0.5454	395	437	570	588
				C	2.9579	-0.6226	-0.7209	608	612	655	686
				C	2.5349	0.6401	-1.1554	712	724	780	832
				C	1.7127	1.4223	-0.3471	873	899	931	960
				C	-0.8143	0.1975	0.2029	968	980	983	990
				C	-1.1325	-1.0934	-0.1668	997	1014	1021	1049
				C	-2.4769	-1.3893	-0.4233	1076	1080	1168	1170
				C	-3.4490	-0.3951	-0.2987	1175	1180	1298	1307
				C	-3.0892	0.8985	0.0800	1315	1323	1429	1443
				C	-1.7462	1.2075	0.3323	1460	1474	1542	1562
				H	1.5136	-0.6746	2.3741	1576	1621	3144	3150

				H	2.9794	-2.0514	0.8988	3154	3160	3160	3165
				H	3.6194	-1.2115	-1.3457	3177	3178	3182	3188
				H	2.8799	1.0304	-2.1073				
				H	1.4204	2.4227	-0.6450				
				H	-0.3706	-1.8616	-0.2531				
				H	-2.7625	-2.3947	-0.7168				
				H	-4.4890	-0.6296	-0.4968				
				H	-3.8480	1.6687	0.1770				
				H	-1.4573	2.2125	0.6248				
TS2	0.178725	A	671.04825	C	-0.7268	-0.0434	-0.0114	-878	64	91	117
		B	3334.04079	C	-1.4522	-1.1958	-0.3725	182	263	281	314
		C	3837.48601	C	-2.8450	-1.2000	-0.3806	369	415	422	502
				C	-3.5625	-0.0566	-0.0300	558	615	620	635
				C	-2.8710	1.1032	0.3355	704	711	750	751
				C	-1.4932	1.0665	0.3246	785	856	860	913
				C	0.7581	-0.0324	-0.0073	933	953	966	985
				C	1.4822	-1.1354	0.4680	990	1002	1013	1020
				C	2.8745	-1.1306	0.4622	1026	1053	1070	1100
				C	3.5704	-0.0229	-0.0191	1130	1179	1182	1205
				C	2.8622	1.0804	-0.4930	1250	1296	1321	1322
				C	1.4701	1.0764	-0.4866	1355	1439	1476	1480
				H	-0.9104	-2.0864	-0.6730	1527	1575	1614	1628
				H	-3.3736	-2.1010	-0.6710	1641	2341	3158	3161
				H	-4.6470	-0.0640	-0.0374	3164	3169	3174	3179
				H	-3.4049	2.0016	0.6272	3186	3187	3193	
				H	-0.8545	2.3017	0.8649				
				H	0.9510	-1.9924	0.8665				
				H	3.4161	-1.9898	0.8424				
				H	4.6545	-0.0189	-0.0235				
				H	3.3945	1.9446	-0.8745				
				H	0.9272	1.9312	-0.8719				
				H	-0.5538	3.0175	1.2125				
TSa	0.173588	A	1207.86033	C	0.7028	-0.3218	0.0547	-1184	51	57	83
		B	3358.15583	C	1.4273	-1.5169	0.2340	104	134	262	300
		C	4354.75361	C	2.8193	-1.5244	0.2370	359	409	418	424
				C	3.5407	-0.3432	0.0662	507	555	615	631
				C	2.8558	0.8639	-0.1131	639	697	710	737
				C	1.4788	0.8184	-0.1134	756	767	781	853
				C	-0.7794	-0.2891	0.0550	860	931	952	984
				C	-1.5215	-1.3160	-0.5453	991	1004	1011	1020
				C	-2.9129	-1.2803	-0.5464	1041	1044	1056	1088
				C	-3.5891	-0.2167	0.0507	1104	1141	1179	1183
				C	-2.8631	0.8107	0.6491	1206	1252	1298	1319
				C	-1.4710	0.7743	0.6555	1323	1356	1448	1475

				H	0.8823	-2.4406	0.3960	1484	1527	1575	1613
				H	3.3464	-2.4600	0.3853	1624	1638	3162	3164
				H	4.6248	-0.3525	0.0728	3167	3172	3176	3182
				H	3.3919	1.7952	-0.2543	3183	3191	3192	
				H	0.8192	2.0064	-0.3835				
				H	-1.0065	-2.1330	-1.0377				
				H	-3.4699	-2.0783	-1.0245				
				H	-4.6727	-0.1886	0.0467				
				H	-3.3791	1.6405	1.1187				
				H	-0.9180	1.5634	1.1526				
				O	0.2819	2.9868	-0.5720				
TSb	0.185631	A	1298.63880	C	0.6474	-0.3613	0.0515	-1291	42	77	83
		B	3373.74805	C	1.2924	-1.5938	0.2749	114	131	153	264
		C	4490.24759	C	2.6795	-1.7026	0.2788	302	335	397	414
				C	3.4782	-0.5827	0.0571	446	504	559	619
				C	2.8714	0.6562	-0.1627	630	646	688	707
				C	1.4899	0.7312	-0.1605	742	759	784	791
				C	-0.8357	-0.2737	0.0375	852	863	927	949
				C	-1.6003	-1.3079	-0.5235	962	985	993	1003
				C	-2.9909	-1.2476	-0.5268	1014	1019	1036	1055
				C	-3.6458	-0.1508	0.0308	1081	1104	1130	1181
				C	-2.8973	0.8866	0.5840	1183	1210	1250	1289
				C	-1.5065	0.8281	0.5866	1313	1323	1360	1386
				H	0.6860	-2.4710	0.4710	1457	1482	1489	1530
				H	3.1387	-2.6672	0.4635	1582	1616	1624	1642
				H	4.5591	-0.6656	0.0545	3161	3163	3170	3172
				H	3.4729	1.5381	-0.3510	3179	3182	3189	3190
				H	1.0001	1.8522	-0.4169	3204	3767		
				H	-1.1029	-2.1544	-0.9831				
				H	-3.5623	-2.0535	-0.9738				
				H	-4.7288	-0.1021	0.0280				
				H	-3.3966	1.7465	1.0162				
				H	-0.9382	1.6448	1.0124				
				O	0.7060	3.0757	-0.4596				
				H	1.3301	3.4359	0.1902				
TS3	0.205317	A	1800.44857	C	0.9390	-0.4193	-0.0655	-308	29	49	66
		B	3517.74237	C	1.5028	0.6223	-0.8174	83	108	133	193
		C	4975.47215	C	2.8788	0.8361	-0.8218	260	306	369	411
				C	3.7196	0.0132	-0.0736	416	430	498	558
				C	3.1722	-1.0250	0.6789	596	617	634	694
				C	1.7961	-1.2392	0.6829	704	713	746	750
				C	-0.5279	-0.6505	-0.0754	782	786	857	863
				C	-2.8237	0.2152	-0.0677	874	933	951	971
				C	-3.3246	-1.0893	-0.1437	988	989	1003	1013

				C	-2.4385	-2.1663	-0.1779	1024	1027	1049	1067
				C	-1.0626	-1.9528	-0.1446	1097	1123	1177	1181
				H	0.8535	1.2506	-1.4163	1201	1243	1295	1319
				H	3.2957	1.6409	-1.4172	1320	1353	1374	1433
				H	4.7909	0.1794	-0.0766	1470	1478	1524	1536
				H	3.8169	-1.6649	1.2711	1571	1612	1624	1639
				H	1.3791	-2.0360	1.2886	3045	3140	3155	3160
				H	-3.4948	1.0659	-0.0219	3161	3167	3172	3177
				H	-4.3959	-1.2589	-0.1719	3183	3185	3190	3240
				H	-2.8204	-3.1791	-0.2412				
				H	-0.3856	-2.7991	-0.2022				
				C	-1.4568	0.3824	-0.0363				
				C	-0.9146	2.4930	0.9107				
				H	0.0591	2.0742	1.1136				
				C	-1.4234	3.4751	0.1834				
				H	-2.4164	3.8788	0.3684				
				H	-0.8992	3.8794	-0.6862				
TS4	0.211355	A	1510.21073	C	-0.9427	-0.3219	0.0197	-863	47	76	86
		B	3626.94321	C	-1.6033	0.5731	0.8500	105	177	196	227
		C	4680.23304	C	-2.9689	0.7619	0.8793	257	289	317	329
				C	-3.7550	0.0068	0.0021	420	428	474	541
				C	-3.1437	-0.9075	-0.8551	567	581	620	626
				C	-1.7597	-1.0734	-0.8461	664	715	729	755
				C	0.5344	-0.5260	0.0427	777	794	811	864
				C	2.8224	0.2375	-0.1551	891	913	938	955
				C	3.2916	-1.0367	0.1353	967	969	994	997
				C	2.3867	-2.0704	0.3729	1012	1022	1028	1043
				C	1.0220	-1.8102	0.3199	1061	1080	1117	1134
				H	-0.8378	1.3214	1.8944	1178	1186	1220	1251
				H	-3.4224	1.4692	1.5657	1281	1306	1315	1324
				H	-4.8324	0.1316	-0.0063	1343	1439	1451	1469
				H	-3.7474	-1.4946	-1.5380	1484	1511	1574	1600
				H	-1.2941	-1.7801	-1.5254	1627	1635	1681	2367
				H	3.5311	1.0249	-0.3833	3137	3156	3157	3163
				H	4.3587	-1.2271	0.1602	3163	3172	3173	3182
				H	2.7404	-3.0706	0.5958	3186	3191	3220	
				H	0.3136	-2.6070	0.5178				
				C	1.4482	0.5260	-0.2010				
				C	0.9780	1.8790	-0.5528				
				H	-0.0162	1.9339	-0.9854				
				C	1.6548	3.0183	-0.3804				
				H	2.6331	3.0520	0.0870				
				H	1.2338	3.9668	-0.6921				
				H	-0.4499	1.7410	2.5214				

TS5	0.199601	A	1309.57873	C	3.4963	-0.5814	-0.0754	-211	75	84	137
		B	3367.31637	C	2.8612	0.6243	-0.3427	152	244	272	317
		C	4535.13640	C	1.4708	0.7649	-0.2196	380	414	422	482
				C	0.6838	-0.3709	0.1045	503	561	585	602
				C	1.3517	-1.5733	0.3931	621	685	704	724
				C	2.7344	-1.6819	0.3160	742	773	781	813
				C	0.8617	2.0862	-0.4467	857	883	902	945
				C	-0.8051	-0.3512	0.0540	964	969	984	989
				C	-1.5754	0.7809	0.2782	993	1020	1041	1057
				C	0.0091	2.6566	0.4266	1072	1117	1143	1178
				C	-2.9491	0.8461	0.2260	1186	1221	1246	1269
				H	-3.4831	1.7712	0.4177	1291	1299	1316	1330
				C	-3.6445	-0.3286	-0.0839	1432	1438	1468	1484
				C	-2.9293	-1.4996	-0.3369	1506	1567	1591	1620
				C	-1.5385	-1.5133	-0.2754	1626	1636	3130	3142
				H	1.0811	2.5844	-1.3882	3152	3159	3162	3168
				H	4.5746	-0.6589	-0.1558	3171	3181	3185	3191
				H	3.4478	1.4922	-0.6255	3225			
				H	0.7748	-2.4398	0.6928				
				H	3.2151	-2.6239	0.5549				
				H	-0.1002	2.2850	1.4375				
				H	-4.7284	-0.3239	-0.1350				
		H	-3.4584	-2.4094	-0.5974						
H	-1.0118	-2.4310	-0.5120								
H	-0.4741	3.6013	0.2027								
TS6	0.194996	A	1152.76480	C	-3.5689	-0.3039	-0.0214	-629	93	99	203
		B	3292.20982	C	-2.8418	0.8658	-0.0696	233	249	298	345
		C	4416.28897	C	-1.4272	0.8480	-0.0507	408	422	437	446
				C	-0.7395	-0.4001	0.0108	506	513	548	557
				C	-1.5144	-1.5786	0.0634	600	631	722	725
				C	-2.8958	-1.5359	0.0486	730	751	767	797
				C	-0.6842	2.0664	-0.0951	840	842	873	880
				C	0.7193	-0.4087	0.0034	887	957	966	987
				C	1.4219	0.8269	-0.0206	992	998	1016	1060
				C	0.6847	2.0682	-0.0175	1061	1113	1164	1167
				C	2.8319	0.8308	-0.0437	1182	1188	1222	1237
				H	3.3503	1.7838	-0.0563	1264	1304	1321	1364
				C	3.5464	-0.3492	-0.0448	1372	1440	1448	1463
				C	2.8597	-1.5744	-0.0203	1488	1528	1556	1605
				C	1.4788	-1.6001	0.0028	1618	1643	1651	3160
				H	-1.2273	3.0035	-0.1526	3161	3164	3170	3171
				H	-4.6525	-0.2761	-0.0337	3181	3184	3187	3194
				H	-3.3485	1.8240	-0.1192	3207			
				H	-1.0276	-2.5435	0.1194				

				H	-3.4621	-2.4594	0.0915				
				H	1.2364	2.9919	-0.1486				
				H	4.6301	-0.3329	-0.0638				
				H	3.4147	-2.5057	-0.0213				
				H	0.9789	-2.5598	0.0155				
				H	0.8822	2.5434	1.8973				
TS7	0.194677	A	1062.12556	C	0.7115	0.1450	-0.7335	-199	-5	21	43
		B	6202.77873	C	-0.1484	-0.8868	-0.5383	65	94	175	199
		C	6576.38449	C	-1.4914	-0.5821	-0.1570	232	328	369	388
				C	-1.8669	0.7910	0.0089	473	482	494	513
				C	-0.9000	1.8099	-0.2091	561	615	623	650
				C	0.3925	1.4972	-0.5782	673	694	744	758
				H	-2.1772	-2.6306	-0.0610	766	790	807	848
				H	0.1507	-1.9234	-0.6604	883	897	931	939
				C	-2.4638	-1.5917	0.0649	957	970	991	996
				C	-3.2016	1.0913	0.3902	1037	1046	1110	1142
				H	-1.1937	2.8473	-0.0788	1160	1172	1208	1250
				C	-4.1204	0.0905	0.5979	1276	1314	1339	1384
				C	-3.7472	-1.2642	0.4335	1392	1440	1456	1464
				H	-3.4867	2.1308	0.5160	1527	1590	1613	1636
				H	-5.1356	0.3357	0.8887	1652	2111	3135	3147
				H	-4.4802	-2.0459	0.6001	3150	3153	3157	3162
				C	3.0535	-0.4234	-1.4291	3173	3174	3186	3238
				H	2.6695	-0.3956	-2.4200	3456			
				C	3.7504	-0.5120	-0.4374				
				C	4.4702	-0.6333	0.7735				
				H	4.4945	-1.6274	1.2136				
				C	5.1078	0.3758	1.3880				
				H	5.1078	1.3798	0.9810				
				H	5.6428	0.2097	2.3149				
				H	1.1302	2.2754	-0.7404				
TS8	0.193965	A	1098.41344	C	-0.8731	1.0534	-0.1298	-1952	56	72	129
		B	4830.22595	C	-0.3072	-0.2014	-0.1587	145	170	218	286
		C	5841.76477	C	1.0601	-0.4593	-0.0595	310	352	422	460
				C	1.9156	0.7005	0.0524	491	500	519	533
				C	1.3348	1.9951	0.0690	592	646	661	678
				C	-0.0299	2.1811	-0.0177	753	757	760	789
				H	1.0007	-2.6199	-0.1542	819	865	876	929
				H	-1.5640	-0.8949	-0.2749	935	958	971	973
				C	1.6490	-1.7551	-0.0702	990	1000	1018	1035
				C	3.3185	0.4964	0.1435	1038	1095	1140	1162
				H	1.9925	2.8538	0.1556	1174	1185	1232	1258
				C	3.8530	-0.7688	0.1316	1305	1313	1367	1371
				C	3.0097	-1.9037	0.0253	1380	1436	1458	1481

				H	3.9662	1.3636	0.2249	1537	1582	1606	1618
				H	4.9261	-0.9054	0.2034	1651	1670	1728	3113
				H	3.4482	-2.8953	0.0176	3137	3155	3157	3159
				C	-2.3452	0.9752	-0.2129	3166	3174	3179	3189
				H	-2.9894	1.8487	-0.2484	3227			
				C	-2.7780	-0.2876	-0.2706				
				C	-4.0270	-0.9866	-0.2806				
				H	-4.1633	-1.7292	-1.0658				
				C	-5.0041	-0.8214	0.6304				
				H	-4.8956	-0.1266	1.4555				
				H	-5.9290	-1.3832	0.5672				
				H	-0.4500	3.1815	0.0072				
TS9	0.195035	A	1196.09194	C	-1.0597	0.8814	-0.2986	-487	57	66	94
		B	4531.10693	C	-0.3221	-0.2985	-0.3987	142	186	240	266
		C	5319.35802	C	1.0483	-0.4598	-0.2082	327	389	415	431
				C	1.7860	0.7313	0.1327	496	508	513	524
				C	1.0732	1.9704	0.2453	578	619	624	653
				C	-0.2710	2.0532	0.0425	722	748	755	761
				H	1.1820	-2.5848	-0.5822	769	817	818	869
				H	-3.4217	-0.4090	-1.9402	919	956	960	971
				C	1.7426	-1.6936	-0.3259	988	988	993	1038
				C	3.1763	0.6281	0.3396	1041	1131	1159	1162
				H	1.6359	2.8626	0.4998	1169	1189	1228	1236
				C	3.8255	-0.5858	0.2189	1266	1327	1344	1387
				C	3.1024	-1.7506	-0.1159	1404	1427	1433	1444
				H	3.7352	1.5224	0.5968	1454	1509	1520	1556
				H	4.8955	-0.6462	0.3815	1607	1629	3100	3107
				H	3.6237	-2.6968	-0.2075	3136	3145	3153	3157
				C	-2.4417	0.9427	-0.5159	3169	3172	3182	3192
				H	-2.9299	1.9147	-0.4556	3238			
				C	-3.2541	-0.2274	-0.8789				
				C	-3.8841	-1.0785	0.0307				
				H	-4.4718	-1.8892	-0.3942				
				C	-3.8303	-0.9787	1.4054				
				H	-3.2582	-0.1987	1.8936				
				H	-4.3549	-1.6849	2.0363				
				H	-0.7831	3.0060	0.1330				
TS11	0.195009	A	1145.00867	C	1.3959	0.8992	0.0132	-627	96	99	223
		B	3292.65329	C	0.7127	-0.3470	-0.0187	224	245	283	351
		C	4410.69391	C	-0.7386	-0.3623	-0.0187	408	413	447	457
				C	-1.4446	0.8759	-0.0057	504	508	553	556
				C	-0.7135	2.1085	0.0221	599	630	719	724
				C	0.6440	2.1200	0.0359	726	747	774	798
				H	-0.9932	-2.5150	-0.0153	832	842	873	885

				H	4.6296	-0.2045	-0.0922	893	960	973	983
				C	-1.4955	-1.5566	-0.0224	992	999	1014	1059
				C	-2.8577	0.8734	-0.0128	1061	1109	1160	1172
				H	-1.2717	3.0388	0.0356	1184	1187	1221	1240
				C	-3.5669	-0.3087	-0.0247	1261	1300	1327	1364
				C	-2.8759	-1.5332	-0.0260	1372	1440	1444	1465
				H	-3.3797	1.8247	-0.0057	1485	1530	1554	1597
				H	-4.6509	-0.2966	-0.0288	1625	1646	1655	3156
				H	-3.4292	-2.4656	-0.0275	3160	3162	3170	3174
				C	2.8101	0.9242	0.0022	3176	3185	3188	3196
				H	3.3126	1.8854	0.0292	3208			
				C	3.5467	-0.2432	-0.0623				
				C	2.8877	-1.4768	-0.1008				
				H	3.4572	-2.3970	-0.1600				
				C	1.4964	-1.5364	-0.0288				
				H	1.3190	-2.0577	1.8649				
				H	1.0157	-2.4940	-0.1753				
				H	1.1866	3.0592	0.0603				
TS14	0.224210	A	2166.16631	C	-3.6370	0.7904	-0.0369	-1049	63	99	123
		B	3586.53199	C	-3.2261	-0.5129	-0.2239	152	186	225	256
		C	5647.20827	C	-1.8629	-0.8758	-0.1454	262	297	349	395
				C	-0.8600	0.1296	0.0579	410	421	480	493
				C	-1.3592	1.4136	0.3320	513	514	540	576
				C	-2.6824	1.7695	0.2985	581	612	672	690
				C	-1.4766	-2.2545	-0.1952	721	736	763	777
				C	0.5488	-0.2479	0.0242	799	816	840	846
				C	0.8608	-1.6401	0.0913	895	920	935	956
				C	-0.1832	-2.6185	-0.0171	973	977	981	987
				C	2.2004	-2.0639	0.2059	1010	1028	1049	1056
				H	2.4083	-3.1260	0.2792	1107	1116	1143	1173
				C	3.2286	-1.1460	0.1900	1191	1196	1226	1250
				C	2.9391	0.2069	-0.0104	1275	1295	1329	1341
				C	1.6311	0.6805	-0.1108	1352	1406	1422	1446
				H	-2.2500	-3.0031	-0.3313	1450	1468	1518	1522
				H	-4.6878	1.0520	-0.0949	1584	1622	1637	1651
				H	-3.9569	-1.2931	-0.4083	1677	2122	3136	3147
				H	-0.6241	2.4061	1.0622	3157	3159	3163	3167
				H	-2.9903	2.7773	0.5568	3176	3179	3182	3193
				H	0.0958	-3.6666	0.0065	3219			
				H	4.2594	-1.4722	0.2694				
				H	3.7552	0.9049	-0.1517				
				C	1.4260	2.0884	-0.5036				
				H	0.5485	2.2809	-1.1140				
				C	2.2293	3.1144	-0.2095				

				H	3.0932	3.0105	0.4382				
				H	2.0273	4.1065	-0.5954				
				H	-0.3368	3.0201	1.6014				
TS15	0.212331	A	1970.83548	C	-3.5029	-0.3570	-0.0993	-238	71	107	154
		B	3378.37695	C	-2.6954	-1.4641	0.0481	204	221	251	300
		C	5276.43851	C	-1.2901	-1.3336	0.0830	386	405	432	455
				C	-0.6850	-0.0434	0.0143	486	499	507	554
				C	-1.5431	1.0958	-0.1065	563	571	622	636
				C	-2.9205	0.9122	-0.1938	691	721	732	758
				C	-0.4716	-2.5106	0.1467	772	801	808	839
				C	0.7731	0.0316	-0.0206	841	891	919	939
				C	1.5477	-1.1737	-0.0027	968	971	974	980
				C	0.8816	-2.4378	0.0962	986	1006	1061	1074
				C	2.9592	-1.1029	-0.0680	1110	1148	1172	1190
				H	3.5231	-2.0296	-0.0533	1193	1224	1254	1256
				C	3.6189	0.1060	-0.1447	1297	1305	1342	1350
				C	2.8748	1.3080	-0.1454	1403	1422	1439	1455
				C	1.5145	1.2146	-0.0854	1468	1507	1522	1581
				C	-0.0461	2.9625	0.5906	1614	1631	1642	1651
				C	-1.0226	2.4687	-0.1952	3133	3145	3151	3155
				H	-1.4281	3.0894	-0.9905	3160	3161	3167	3174
				H	0.3416	3.9629	0.4335	3177	3186	3227	
				H	-0.9676	-3.4730	0.2156				
				H	-4.5807	-0.4636	-0.1464				
				H	-3.1282	-2.4566	0.1139				
				H	-3.5541	1.7845	-0.3156				
				H	1.4847	-3.3395	0.1281				
				H	4.7023	0.1388	-0.1953				
				H	3.3808	2.2671	-0.1899				
				H	0.2703	2.4613	1.4959				
TS16	0.207579	A	1827.13716	C	3.5292	0.0089	-0.0212	-629	96	147	196
		B	3264.93038	C	2.8286	1.2107	-0.0524	237	251	299	346
		C	5063.68577	C	1.4245	1.2234	-0.0417	358	410	420	461
				C	0.7204	-0.0189	-0.0027	498	506	508	516
				C	1.4470	-1.2446	0.0230	550	554	582	594
				C	2.8502	-1.2055	0.0165	685	703	723	748
				C	0.6719	2.4386	-0.0779	762	772	813	814
				C	-0.7063	-0.0336	-0.0059	826	832	862	906
				C	-1.4363	1.1892	-0.0290	919	977	979	984
				C	-0.6998	2.4335	-0.0133	988	997	1014	1090
				C	-2.8348	1.1497	-0.0553	1113	1124	1157	1166
				H	-3.3916	2.0806	-0.0685	1197	1203	1227	1258
				C	-3.5119	-0.0679	-0.0545	1262	1265	1342	1349
				C	-2.8091	-1.2677	-0.0225	1396	1418	1431	1456

				C	-1.4062	-1.2764	0.0016	1458	1478	1503	1531
				C	-0.6456	-2.4944	0.0332	1581	1619	1625	1632
				C	0.7134	-2.4795	0.0462	1659	3157	3160	3160
				H	1.2713	-3.4098	0.0694	3164	3168	3169	3176
				H	-1.1829	-3.4370	0.0454	3181	3185	3185	
				H	1.2084	3.3804	-0.1207				
				H	4.6134	0.0185	-0.0268				
				H	3.3655	2.1529	-0.0831				
				H	3.4049	-2.1376	0.0379				
				H	-0.9088	2.8926	1.9121				
				H	-4.5958	-0.0796	-0.0748				
				H	-3.3443	-2.2114	-0.0167				
				H	-1.2519	3.3577	-0.1391				
TS17	0.203719	A	2087.36762	C	0.9892	-0.4593	-0.7443	-192	9	20	42
		B	6530.46861	C	0.0224	0.4730	-0.5434	57	92	110	142
		C	7840.18963	C	-1.2715	0.0243	-0.1438	177	210	231	329
				C	-1.4881	-1.3807	0.0324	357	362	437	441
				C	-0.4164	-2.2873	-0.1940	480	490	530	562
				C	0.8286	-1.8367	-0.5801	571	588	631	644
				H	0.2003	1.5347	-0.6730	650	675	694	696
				C	-2.3628	0.9273	0.0905	700	747	774	787
				C	-2.7697	-1.8399	0.4316	827	860	873	898
				H	-0.5947	-3.3495	-0.0559	926	942	961	985
				H	1.6469	-2.5275	-0.7495	997	1024	1054	1093
				C	-3.7995	-0.9557	0.6499	1111	1151	1190	1218
				C	-3.5968	0.4273	0.4796	1241	1278	1315	1327
				H	-2.9249	-2.9057	0.5625	1359	1386	1440	1446
				H	-4.7750	-1.3166	0.9546	1469	1513	1593	1609
				H	-4.4127	1.1185	0.6532	1635	1637	2114	2194
				C	-2.1888	2.3336	-0.0740	3135	3148	3153	3163
				C	-2.0482	3.5231	-0.2117	3172	3176	3180	3194
				H	-1.9289	4.5721	-0.3312	3239	3456	3475	
				C	3.2653	0.3611	-1.4292				
				H	2.7956	0.6170	-2.3480				
				C	4.0360	0.1942	-0.5049				
				C	4.8687	-0.0684	0.6074				
				H	5.4289	-0.9999	0.5738				
				C	5.0046	0.7458	1.6661				
				H	4.4629	1.6814	1.7358				
				H	5.6637	0.4843	2.4847				
TS18	0.202777	A	2058.59861	C	-0.9494	-1.4321	-0.1456	-1956	44	59	99
		B	4855.54177	C	-0.3547	-0.1888	-0.1343	112	146	156	179
		C	6824.05807	C	1.0160	0.0318	-0.0287	221	285	304	339
				C	1.8444	-1.1490	0.0449	387	437	452	470

				C	1.2334	-2.4297	0.0217	506	525	534	588
				C	-0.1348	-2.5822	-0.0695	588	594	632	669
				H	-1.5898	0.5381	-0.2286	681	691	736	745
				C	1.6397	1.3270	0.0003	757	781	831	874
				C	3.2513	-0.9913	0.1401	884	925	930	961
				H	1.8725	-3.3043	0.0803	963	981	999	1003
				H	-0.5777	-3.5729	-0.0762	1038	1055	1088	1098
				C	3.8217	0.2588	0.1668	1159	1182	1190	1238
				C	3.0176	1.4166	0.0983	1253	1292	1311	1346
				H	3.8729	-1.8792	0.1934	1364	1394	1435	1451
				H	4.8978	0.3654	0.2408	1463	1532	1582	1606
				H	3.4805	2.3957	0.1211	1614	1635	1668	1731
				C	0.8428	2.5066	-0.0693	2196	3115	3137	3157
				C	0.1777	3.5103	-0.1278	3160	3161	3176	3179
				H	-0.4089	4.3947	-0.1772	3194	3227	3476	
				C	-2.4185	-1.3148	-0.2284				
				H	-3.0847	-2.1698	-0.2924				
				C	-2.8153	-0.0388	-0.2466				
				C	-4.0448	0.6937	-0.2393				
				H	-4.1544	1.4667	-0.9987				
				C	-5.0309	0.5240	0.6609				
				H	-4.9458	-0.2011	1.4623				
				H	-5.9391	1.1138	0.6139				
TS19	0.208177	A	2192.56852	C	-1.4364	-1.1783	-0.1892	-275	36	82	127
		B	3756.43505	C	-0.6267	-0.0659	-0.1205	137	178	197	208
		C	5870.12516	C	0.7756	-0.0840	-0.0352	289	327	370	402
				C	1.4016	-1.3801	0.0341	407	450	478	489
				C	0.5845	-2.5419	-0.0338	513	542	575	589
				C	-0.7745	-2.4502	-0.1485	611	633	675	681
				C	1.6209	1.0787	-0.0157	697	708	752	765
				C	2.8079	-1.4742	0.1572	798	802	834	843
				H	1.0639	-3.5142	0.0036	911	925	933	964
				H	-1.3777	-3.3512	-0.2046	965	982	984	996
				C	3.5897	-0.3431	0.1968	1039	1082	1095	1171
				C	2.9966	0.9279	0.1033	1173	1195	1225	1243
				H	3.2605	-2.4585	0.2200	1259	1286	1316	1352
				H	4.6663	-0.4236	0.2925	1380	1423	1445	1458
				H	3.6174	1.8154	0.1182	1474	1509	1552	1582
				C	1.1003	2.4007	-0.1371	1612	1622	1649	2193
				C	0.7458	3.5471	-0.2526	3123	3134	3151	3155
				H	0.4204	4.5532	-0.3565	3158	3161	3175	3180
				C	-2.8967	-1.1755	-0.2268	3195	3248	3474	
				H	-3.3487	-2.1396	-0.4427				
				C	-3.7233	-0.1677	0.1516				

				C	-3.2644	1.1450	0.5287				
				H	-3.7245	1.6058	1.4007				
				C	-2.2375	1.7769	-0.0956				
				H	-1.9513	1.5196	-1.1062				
				H	-1.8291	2.6998	0.2932				
				H	-4.7775	-0.3995	0.2826				
TS20	0.206248	A	2131.69932	C	-3.5412	0.4710	-0.1917	-1991	70	121	159
		B	3307.37061	C	-3.0376	-0.8276	-0.2818	204	225	264	303
		C	5353.83143	C	-1.6616	-1.0862	-0.0607	338	378	415	444
				C	-0.8023	-0.0102	0.2470	492	500	512	521
				C	-1.3474	1.3163	0.5087	551	561	580	596
				C	-2.7402	1.5198	0.2384	625	651	699	712
				C	-1.1002	-2.4039	-0.1507	730	738	771	788
				C	0.6120	-0.1845	0.1747	808	833	858	863
				C	1.1478	-1.5056	0.0999	923	965	972	977
				C	0.2393	-2.6083	-0.0154	985	988	1007	1047
				C	2.5439	-1.6815	0.0640	1095	1120	1157	1171
				H	2.9490	-2.6877	0.0434	1190	1212	1227	1248
				C	3.3886	-0.5858	0.0147	1264	1310	1337	1340
				C	2.8642	0.7105	-0.0511	1362	1402	1415	1439
				C	1.4904	0.9341	0.0266	1452	1479	1516	1531
				H	-1.7685	-3.2412	-0.3231	1562	1586	1617	1638
				H	-4.5927	0.6489	-0.3903	1850	3045	3158	3160
				H	-3.6961	-1.6514	-0.5342	3163	3173	3177	3179
				H	-0.9780	1.8194	1.4057	3184	3192	3371	
				H	-3.1801	2.4911	0.4356				
				H	0.6484	-3.6123	-0.0575				
				H	4.4629	-0.7286	-0.0150				
				H	3.5232	1.5606	-0.1801				
				H	-0.4149	2.0653	-0.2001				
				C	0.9588	2.2742	-0.2066				
				C	1.3113	3.4739	-0.3527				
				H	1.0929	4.4992	-0.5639				
TS21	0.211518	A	1906.44019	C	-3.5651	0.0378	0.0260	-352	93	132	163
		B	3375.99994	C	-2.8776	-1.1272	-0.2706	221	226	278	300
		C	5123.53423	C	-1.4672	-1.1837	-0.1645	389	414	434	477
				C	-0.7443	-0.0089	0.1703	495	504	513	550
				C	-1.4773	1.1457	0.5885	574	594	603	658
				C	-2.8751	1.1533	0.5113	673	720	727	757
				C	-0.7548	-2.4194	-0.3103	772	779	810	831
				C	0.6972	-0.0232	0.1200	838	870	876	890
				C	1.3611	-1.2837	0.0841	917	920	972	977
				C	0.5893	-2.4761	-0.1159	983	1008	1038	1062
				C	2.7693	-1.3381	0.1736	1105	1139	1168	1175

				H	3.2579	-2.3066	0.1851	1189	1222	1223	1246
				C	3.5133	-0.1772	0.2110	1258	1284	1331	1346
				C	2.8717	1.0613	0.0703	1365	1415	1438	1458
				C	1.4852	1.1658	-0.0065	1465	1518	1535	1581
				H	-1.3186	-3.3196	-0.5313	1605	1619	1640	1645
				H	-4.6466	0.0627	-0.0507	3038	3157	3159	3160
				H	-3.4169	-2.0227	-0.5605	3166	3170	3176	3180
				H	-0.9982	1.8446	1.2601	3185	3188	3219	
				H	-3.4243	2.0175	0.8677				
				H	1.1124	-3.4255	-0.1608				
				H	4.5942	-0.2200	0.2819				
				H	3.4695	1.9612	-0.0319				
				C	0.9212	2.4605	-0.4389				
				C	-0.3538	2.7728	-0.5792				
				H	-0.8641	3.6627	-0.9208				
				H	1.6763	3.1875	-0.7543				
TS22	0.208065	A	1807.55685	C	-3.5332	-0.0240	-0.0231	-1015	95	148	208
		B	3269.55111	C	-2.8595	1.1913	-0.0016	236	262	350	395
		C	5048.17056	C	-1.4559	1.2335	0.0128	403	441	459	493
				C	-0.7266	0.0070	0.0164	503	505	519	534
				C	-1.4279	-1.2362	-0.0214	545	561	584	596
				C	-2.8267	-1.2268	-0.0389	688	698	721	747
				C	-0.7229	2.4670	0.0173	750	774	809	812
				C	0.6945	0.0271	0.0298	828	838	859	899
				C	1.3961	1.2626	0.0026	914	975	976	982
				C	0.6371	2.4814	0.0043	984	990	1010	1089
				C	2.8012	1.2517	-0.0481	1112	1122	1164	1167
				H	3.3360	2.1950	-0.0740	1194	1202	1221	1250
				C	3.5062	0.0488	-0.1109	1261	1265	1334	1345
				C	2.8426	-1.1659	-0.0611	1389	1425	1430	1447
				C	1.4315	-1.2119	0.1195	1455	1472	1511	1524
				C	0.6864	-2.4533	-0.0209	1583	1609	1621	1640
				C	-0.6654	-2.4586	-0.0723	1665	3157	3159	3161
				H	-1.2048	-3.3960	-0.1591	3162	3168	3172	3176
				H	1.2464	-3.3816	-0.0542	3179	3185	3186	
				H	-1.2800	3.3981	0.0215				
				H	-4.6172	-0.0383	-0.0347				
				H	-3.4165	2.1223	0.0005				
				H	-3.3626	-2.1697	-0.0690				
				H	1.1748	3.4238	-0.0060				
				H	4.5863	0.0663	-0.2044				
				H	3.3953	-2.0979	-0.1008				
				H	1.4770	-1.2840	1.8538				
TS23	0.204130	A	2113.11016	C	-0.9851	-1.4892	-0.1654	-273	11	27	51

		B	5190.55442	C	-0.3695	-0.2771	-0.1114	98	119	144	164
		C	7202.28323	C	1.0258	-0.0929	-0.0266	174	203	233	341
				C	1.8187	-1.2991	0.0073	360	368	439	458
				C	1.1761	-2.5638	-0.0492	483	485	543	559
				C	-0.1898	-2.6630	-0.1351	577	591	627	639
				C	1.7138	1.1680	0.0262	641	685	704	710
				C	3.2309	-1.2062	0.0965	745	753	760	799
				H	1.7916	-3.4566	-0.0230	816	865	900	902
				H	-0.6698	-3.6350	-0.1777	927	933	976	987
				C	3.8582	0.0141	0.1492	996	1019	1064	1098
				C	3.0991	1.1973	0.1130	1111	1163	1188	1202
				H	3.8092	-2.1240	0.1221	1236	1260	1310	1345
				H	4.9381	0.0747	0.2171	1355	1383	1437	1453
				H	3.5967	2.1585	0.1519	1465	1511	1582	1616
				C	1.0331	2.4220	-0.0107	1623	1645	2071	2190
				C	0.5466	3.5253	-0.0384	3130	3146	3158	3162
				H	0.1089	4.4934	-0.0660	3174	3180	3184	3196
				H	-2.0640	-1.5685	-0.2264	3238	3408	3471	
				C	-2.1646	1.3590	-0.1198				
				H	-1.4171	2.1128	-0.0335				
				C	-3.2500	0.8087	-0.2061				
				C	-4.4421	0.0687	-0.3448				
				H	-4.7870	-0.0951	-1.3637				
				C	-5.1634	-0.4225	0.6802				
				H	-4.8575	-0.2773	1.7094				
				H	-6.0754	-0.9782	0.4997				
TS24	0.202104	A	2099.36290	C	-0.2826	-2.2159	-0.1023	-1725	36	57	92
		B	4585.77019	C	-0.3114	-0.8300	-0.0996	121	154	183	222
		C	6580.90465	C	0.9164	-0.0931	-0.0213	235	304	321	340
				C	2.1483	-0.8200	0.0518	374	396	474	494
				C	2.1239	-2.2381	0.0457	509	533	548	552
				C	0.9331	-2.9199	-0.0297	577	590	638	647
				C	0.9628	1.3390	-0.0140	660	719	755	772
				C	3.3733	-0.1095	0.1292	776	804	828	853
				H	3.0644	-2.7756	0.1022	877	885	908	918
				H	0.9222	-4.0040	-0.0337	935	967	983	991
				C	3.3890	1.2650	0.1347	1019	1048	1103	1107
				C	2.1847	1.9877	0.0630	1155	1189	1202	1239
				H	4.2991	-0.6720	0.1845	1253	1288	1296	1365
				H	4.3296	1.8008	0.1944	1377	1388	1429	1457
				H	2.1980	3.0710	0.0672	1481	1499	1533	1568
				C	-0.2764	2.1018	-0.0887	1607	1623	1644	1832
				C	-0.6932	3.2985	-0.1140	2032	3113	3147	3162
				H	-1.5334	3.9618	-0.1651	3165	3178	3179	3191

				H	-1.2193	-2.7573	-0.1618	3192	3242	3344	
				C	-1.5808	-0.1293	-0.1769				
				H	-1.2125	1.2030	-0.1481				
				C	-2.8264	-0.2614	-0.2497				
				C	-4.2088	-0.1702	-0.3599				
				H	-4.6089	-0.1605	-1.3731				
				C	-5.0786	-0.1172	0.6838				
				H	-4.7330	-0.1306	1.7103				
				H	-6.1457	-0.0605	0.5104				
TS26	0.206637	A	1678.59816	C	0.5185	1.8837	-0.1282	-2060	53	78	126
		B	4361.71709	C	0.3110	0.5261	-0.1171	164	180	203	252
		C	5959.88990	C	-0.9749	-0.0191	-0.0298	320	360	395	450
				C	-2.0846	0.8670	0.0722	458	481	497	507
				C	-1.8333	2.2639	0.0904	531	552	596	627
				C	-0.5379	2.7806	0.0040	632	684	693	746
				C	-1.1239	-1.4384	-0.0470	758	771	801	805
				C	-3.3798	0.2775	0.1559	835	836	907	911
				H	-2.6743	2.9464	0.1636	920	951	981	990
				H	-0.3835	3.8540	0.0189	998	1024	1046	1062
				C	-3.5238	-1.0919	0.1378	1085	1128	1144	1169
				C	-2.4059	-1.9565	0.0353	1179	1203	1237	1253
				H	-4.2524	0.9172	0.2349	1309	1315	1350	1381
				H	-4.5158	-1.5252	0.2016	1418	1435	1440	1451
				H	-2.5611	-3.0302	0.0169	1469	1518	1573	1581
				C	0.0862	-2.2468	-0.1658	1596	1597	1632	1652
				C	1.3380	-1.7203	-0.2361	1711	3110	3137	3156
				H	2.2000	-2.3711	-0.3246	3157	3160	3168	3175
				H	1.9439	1.7316	-0.2497	3183	3186	3227	
				C	1.5244	-0.2831	-0.1885				
				H	-0.0378	-3.3250	-0.1971				
				C	2.6242	0.5106	-0.2277				
				C	4.0398	0.3798	-0.1570				
				H	4.6225	1.0634	-0.7736				
				C	4.7038	-0.4925	0.6320				
				H	4.1808	-1.1611	1.3063				
				H	5.7864	-0.5438	0.6193				
TS27	0.211684	A	1802.24157	C	-1.1395	1.3775	0.0608	-148	54	118	169
		B	3736.80475	C	-0.6211	0.1029	0.0480	197	216	242	296
		C	5497.45166	C	0.8166	0.0182	-0.0029	377	394	434	460
				C	1.6029	1.2119	-0.0490	471	480	503	533
				C	0.9600	2.4770	-0.0430	543	585	616	642
				C	-0.4180	2.5626	0.0245	656	680	757	764
				C	1.4759	-1.2487	0.0341	772	774	798	822
				C	3.0184	1.1037	-0.0862	833	877	891	909

				H	1.5659	3.3771	-0.0820	953	962	973	980
				H	-0.9147	3.5272	0.0389	987	1010	1050	1094
				C	3.6342	-0.1279	-0.0597	1117	1140	1152	1182
				C	2.8653	-1.3020	0.0063	1201	1233	1240	1262
				H	3.6095	2.0122	-0.1305	1309	1320	1362	1376
				H	4.7159	-0.1956	-0.0852	1412	1432	1445	1457
				H	3.3580	-2.2683	0.0356	1480	1500	1527	1579
				C	0.6640	-2.4413	0.1080	1607	1614	1627	1654
				C	-0.6859	-2.3804	0.1115	3109	3130	3145	3152
				H	-1.2657	-3.2966	0.1489	3156	3160	3167	3169
				C	-1.4219	-1.1325	0.0451	3176	3185	3234	
				H	1.1671	-3.4016	0.1521				
				C	-2.7842	-1.2023	-0.1551				
				C	-3.7317	-0.1363	-0.3243				
				H	-4.5329	-0.3364	-1.0349				
				C	-3.7279	1.0659	0.2966				
				H	-4.4522	1.8280	0.0299				
				H	-3.1147	1.2653	1.1636				
				H	-3.1778	-2.2021	-0.3246				
TS28	0.207480	A	1804.91214	C	-3.5498	-0.0598	0.0199	-560	96	144	207
		B	3299.13279	C	-2.8851	1.1633	0.0312	225	254	293	316
		C	5075.30141	C	-1.4832	1.2178	0.0182	363	410	412	462
				C	-0.7432	-0.0015	-0.0047	497	506	508	509
				C	-1.4320	-1.2502	-0.0178	544	553	585	595
				C	-2.8354	-1.2540	-0.0053	688	701	720	747
				C	-0.7615	2.4586	0.0243	760	780	811	814
				C	0.6818	0.0276	-0.0151	821	833	856	910
				C	1.3698	1.2780	-0.0195	934	977	979	982
				C	0.5990	2.4864	0.0039	986	993	1011	1084
				C	2.7763	1.2841	-0.0604	1109	1128	1166	1167
				H	3.2989	2.2345	-0.0843	1197	1204	1226	1254
				C	3.4924	0.0988	-0.0773	1260	1267	1343	1349
				C	2.8306	-1.1380	-0.0228	1398	1421	1434	1453
				C	1.4187	-1.1909	-0.0381	1457	1484	1504	1528
				C	0.7010	-2.4302	-0.0550	1582	1618	1622	1635
				C	-0.6595	-2.4595	-0.0457	1657	3157	3158	3161
				H	-1.1862	-3.4080	-0.0574	3164	3168	3174	3176
				H	1.2679	-3.3551	-0.0686	3177	3185	3189	
				H	-1.3273	3.3843	0.0428				
				H	-4.6337	-0.0823	0.0299				
				H	-3.4505	2.0890	0.0492				
				H	-3.3621	-2.2023	-0.0156				
				H	1.1265	3.4346	0.0047				
				H	4.5756	0.1214	-0.1097				

H	3.3926	-2.0570	-0.1404
H	3.1786	-1.5415	1.9357
