

Supplementary Materials for

Gas-Phase Synthesis of Racemic Helicenes and their Potential Role in the Enantiomeric Enrichment of Sugars and Amino Acids in Meteorites

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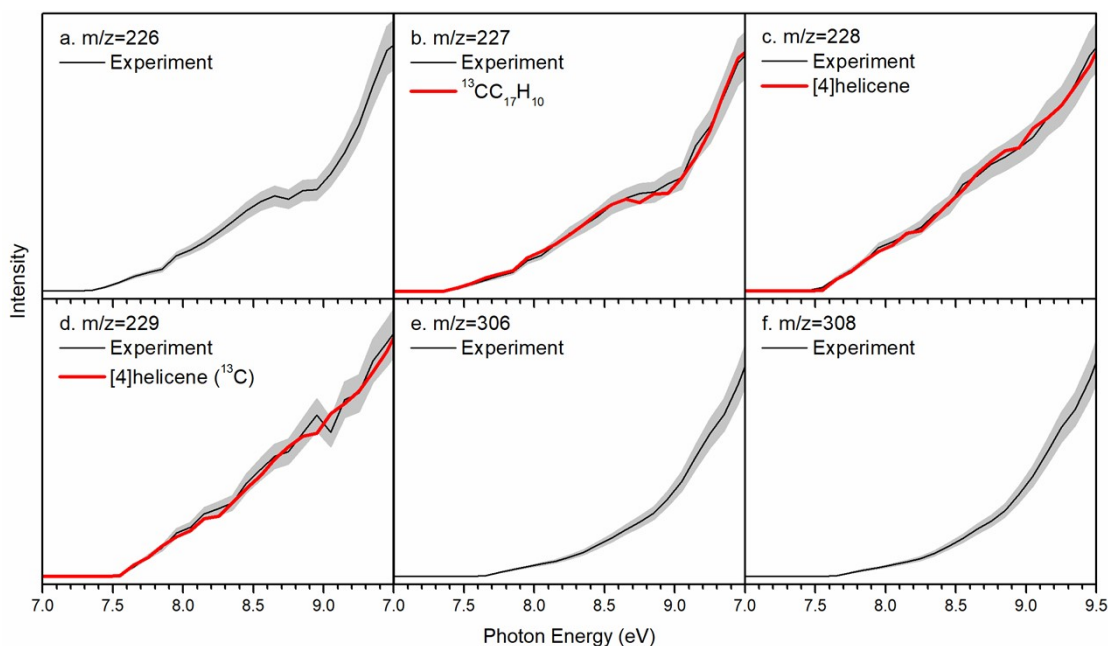
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Fig. S1.



Photoionization efficiency (PIE) curves for reaction of 2-bromobenzo[*c*]phenanthrene - bromo[4]-helicene ($C_{18}H_{11}Br$) - vinylacetylene (C_4H_4). Black: experimentally derived PIE curves; red lines: reference PIE curves. The overall error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a 1σ error of the PIE curve averaged over the individual scans. The PIE curves for $m/z = 308$ and 306 are superimposable and can be connected to 2-bromobenzo[*c*]phenanthrene: $C_{18}H_{11}^{79}Br^+$ ($m/z = 306$) and $C_{18}H_{11}^{71}Br^+$ ($m/z = 308$). Likewise, the PIE graphs for $m/z = 229$ and 228 essentially overlap. Both PIE curves can be replicated through a reference PIE for [4]helicene ($C_{18}H_{12}$; $m/z = 228$) and ^{13}C -[4]helicene ($^{13}CC_{17}H_{12}$; $m/z = 229$). Finally, the PIE curves at $m/z = 226$ and 227 also overlap.

Table S1.

Optimized Cartesian coordinates and calculated vibrational frequencies of various structures involved in the [4]/[5]helicenyl plus vinylacetylene reactions.

Structure	Cartesian Coordinates, Å			Frequencies, cm ⁻¹			
[i1]	C	-2.385414	0.686641	0.006817	5.7183	9.9521	11.2011
	C	-3.803768	0.634145	0.190151	25.3016	33.7357	46.3059
	C	-1.821292	1.964876	-0.241862	80.4067	84.5265	129.8663
	C	-1.629229	-0.556218	-0.015088	178.4983	211.5812	228.0577
	C	-4.468573	1.832656	0.269927	260.6443	279.0589	319.2188
	C	-2.578295	3.116835	-0.193385	325.2711	378.1449	411.3631
	C	-2.353445	-1.766223	-0.142970	438.3684	441.1753	477.4842
	C	-3.951319	3.059498	0.102053	511.3366	525.6124	526.7687
	C	-3.775619	-1.774603	-0.008000	552.6375	559.6069	575.1462
	C	-0.182830	-0.646285	0.087736	592.9689	623.2409	645.1824
	C	-1.673016	-2.993347	-0.407261	672.0826	680.9936	686.3094
	C	0.468167	-1.884486	-0.224699	703.4770	703.8604	749.2939
	C	-0.319119	-3.040246	-0.508006	757.5318	759.7134	780.4124
	C	1.880072	-1.989748	-0.179721	805.0030	824.7806	828.4965
	C	2.674663	-0.932326	0.223973	851.1921	855.8644	876.4762
	C	0.648279	0.403437	0.588882	892.3387	895.4254	958.0447
	C	1.992113	0.210307	0.612933	958.2770	964.6310	967.1520
	C	5.270168	2.209989	-0.803122	975.3878	982.7567	1001.5523
	C	6.411837	1.542090	-0.607524	1009.5098	1012.7253	1057.2972
	C	6.563377	0.448140	0.289942	1078.3746	1112.5044	1123.5548
	C	6.733127	-0.480131	1.039370	1147.1293	1171.2662	1175.3405
	H	-0.784964	2.044144	-0.532471	1183.8721	1205.1928	1223.5573
	H	-5.620208	1.762980	0.437913	1235.4304	1246.1712	1263.7554
	H	-5.543604	-0.647628	0.358594	1307.8527	1322.1524	1343.0992
	H	-2.110436	4.071879	-0.404455	1351.1593	1369.2208	1394.4673
	H	-4.537000	3.969972	0.156607	1410.5434	1440.0933	1446.2112
	H	-4.289663	-2.728179	-0.064307	1451.8173	1471.9905	1498.9977
	H	-2.267926	-3.889236	-0.548717	1530.3881	1545.4483	1588.3683
	H	0.187224	-3.968724	-0.748766	1611.4552	1635.7873	1647.8337
	H	2.336811	-2.936579	-0.451449	1665.3080	1668.2635	2202.1090
	H	3.755303	-1.007772	0.257056	3135.1571	3144.2610	3153.6236
	H	0.211164	1.303394	0.996498	3157.3575	3159.4729	3161.0450
H	5.225934	3.034435	-1.504446	3169.8949	3176.7392	3179.2112	
H	4.359059	1.951279	-0.276346	3181.4241	3186.2930	3201.7969	
H	7.305148	1.829699	-1.156602	3227.3863	3233.8016	3476.1453	
H	6.876944	-1.291954	1.709324				
[i2]	C	0.430177	-1.335679	0.197596	7.5397	12.8417	20.9298
	C	0.786312	-2.721109	0.243104	26.3244	31.1046	51.2538
	C	-0.954605	-1.030043	0.248157	80.6381	85.3721	129.3097
	C	1.478047	-0.344210	0.006872	178.6144	211.8463	226.9192
	C	-0.207345	-3.698049	0.484982	260.6936	278.6879	320.1681
	C	2.129238	-3.117097	-0.031338	325.1794	378.0490	411.5998
	C	-1.908157	-2.006038	0.451055	438.3079	441.0495	477.8265
	C	2.751832	-0.801095	-0.410065	510.5000	525.4634	526.9800
	C	-1.532981	-3.351501	0.608736	552.2654	557.6400	574.4150
	C	3.055454	-2.197002	-0.405982	593.5149	623.0263	671.5965
	C	1.314206	1.083509	0.219308	679.7437	686.7151	703.0625
	C	3.749646	0.125881	-0.838805	703.9643	706.0716	747.6788
	C	2.318947	1.986495	-0.260030	758.0892	759.4220	777.1093
	C	3.520764	1.464823	-0.825009	806.6078	824.5121	826.7659
	C	2.163523	3.386335	-0.109271	851.2242	855.2223	878.4794
	C	1.078175	3.927821	0.554727	892.2184	898.7005	952.2733
	C	0.250103	1.658124	0.981776	954.1869	958.0607	967.1468
	C	0.184984	3.010477	1.087450	975.9231	983.3366	1007.3490
	C	-3.469633	2.249419	0.029648	1010.4228	1013.8794	1056.9460
	C	-4.440972	1.564596	-0.170160	1078.3606	1111.6480	1122.1765
	C	-5.608835	0.777584	-0.372151	1145.4276	1171.6603	1174.6695
	C	-5.722464	-0.189091	-1.289562	1184.3819	1205.1686	1223.2123
	H	-1.292705	-0.021155	0.068442	1235.6295	1245.5450	1263.8811
	H	0.095913	-4.738317	0.542068	1307.5352	1320.9958	1342.6090
	H	2.379847	-4.171704	0.010399	1351.0637	1369.0777	1394.3159
	H	-2.955617	-1.727570	0.470042	1409.9720	1439.3551	1443.6122

	H	-2.285583	-4.111307	0.786041	1451.6742	1471.6733	1498.2693
	H	4.057025	-2.504303	-0.687227	1530.2160	1545.3158	1588.2002
	H	4.693932	-0.268024	-1.198988	1610.7886	1635.4715	1647.3479
	H	4.269539	2.159547	-1.189739	1665.1277	1666.3604	2200.8038
	H	2.933043	4.038510	-0.510869	3134.7248	3146.3025	3154.1710
	H	0.958158	4.998657	0.669061	3157.1686	3159.3581	3161.1382
	H	-0.452044	1.027440	1.507434	3172.7092	3176.7718	3179.3026
	H	-2.601110	2.840665	0.197228	3181.8053	3186.8767	3203.4352
	H	-6.450597	1.001778	0.278696	3230.2254	3235.5035	3454.8819
	H	-4.905579	-0.437963	-1.956490			
	H	-6.642710	-0.751154	-1.392314			
p2	C	-1.584885	-0.368310	0.189299	65.0183	71.7766	90.1923
	C	-2.961122	-0.305922	-0.187919	121.1340	169.4430	174.6380
	C	-1.165325	-1.512612	0.912787	229.2821	245.9173	275.9626
	C	-0.722475	0.782154	-0.054874	312.8460	343.1501	399.0500
	C	-3.800847	-1.424617	0.027396	420.0448	420.9253	451.1723
	C	-2.014086	-2.572040	1.149200	471.3168	477.4819	496.2063
	C	-1.365261	2.017949	-0.331427	527.0924	537.3847	545.3051
	C	-3.337820	-2.547753	0.672475	552.1590	576.6696	611.3338
	C	-2.748081	2.045648	-0.694572	635.1522	659.9005	679.1740
	C	0.722491	0.782080	0.055069	691.7067	724.6865	736.0635
	C	-0.648187	3.240027	-0.208658	753.5254	765.7199	779.0054
	C	1.365397	2.017841	0.331468	785.5749	798.3978	805.1901
	C	0.648433	3.239972	0.208599	817.2553	840.1081	856.5633
	C	2.748241	2.045490	0.694526	866.7740	884.2181	884.9030
	C	3.502166	0.916066	0.691112	937.6227	949.7448	960.8174
	C	1.584861	-0.368436	-0.189183	967.4285	969.4292	978.1861
	C	2.961131	-0.306073	0.187869	981.4815	997.5197	998.7557
	C	1.165107	-1.512755	-0.912514	1047.2512	1058.7675	1082.8936
	C	2.013832	-2.572199	-1.149041	1094.7569	1151.2859	1166.2608
	C	3.337674	-2.547866	-0.672696	1171.9946	1179.5497	1183.4292
	C	3.800806	-1.424741	-0.027639	1184.6747	1207.9627	1225.0696
	H	-0.159857	-1.550366	1.305784	1234.3876	1239.0666	1249.2464
	H	-4.834694	-1.364027	-0.296461	1286.0935	1297.8467	1343.8618
	H	-4.543626	0.941837	-0.993011	1357.0025	1364.7573	1374.2517
	H	-1.659145	-3.424962	1.716611	1398.0421	1412.0161	1448.1889
	H	-3.995068	-3.392516	0.844626	1448.7082	1466.1003	1472.5462
	H	-3.182088	2.998918	-0.977139	1515.1134	1526.5749	1547.0843
	H	-1.172426	4.171147	-0.394752	1555.0192	1590.2931	1623.0281
	H	1.172769	4.171059	0.394592	1647.5104	1649.1120	1655.7888
	H	3.182296	2.998752	0.977062	1661.4907	3157.4521	3157.8519
	H	4.543764	0.941639	0.992884	3159.6895	3160.2138	3162.1974
	H	0.159534	-1.550531	-1.305244	3170.8120	3170.9482	3176.9954
	H	1.658755	-3.425233	-1.716206	3177.8707	3180.7635	3186.2770
H	3.994964	-3.392528	-0.845178	3186.5756	3217.8432	3218.5106	
H	4.834757	-1.364078	0.295886				
p1	C	-2.045629	-0.506256	0.093042	57.0800	63.5956	90.6676
	C	-3.429126	-0.307476	-0.222742	122.5918	154.5401	196.5787
	C	-1.679372	-1.793305	0.570820	218.0040	255.3773	289.3989
	C	-1.133592	0.619141	0.006482	309.4124	321.8994	399.9702
	C	-4.324290	-1.403875	-0.197280	404.0620	415.6479	438.8257
	C	-3.910538	1.005298	-0.491084	473.6963	483.7897	503.7550
	C	-2.580686	-2.834385	0.621322	523.5619	531.5439	538.6028
	C	-1.691292	1.910794	-0.106925	572.1504	589.4655	601.3448
	C	-3.910544	-2.653480	0.198229	636.8863	651.1020	663.9033
	C	-3.081594	2.077757	-0.373480	713.7306	717.9230	747.3337
	C	0.325432	0.509608	0.028727	756.3666	763.0430	775.7166
	C	-0.869881	3.077267	0.060062	790.2634	806.5512	810.2426
	C	1.111821	1.702154	0.256635	818.0069	842.2834	846.8700
	C	0.458206	2.977194	0.301421	859.9764	883.3713	902.6825
	C	2.499971	1.620540	0.340908	916.9969	926.6146	949.7424
	C	3.188879	0.417830	0.139346	964.8218	968.2832	977.7305
	C	1.024629	-0.665156	-0.257018	982.5310	995.0028	1003.7684
	C	2.426363	-0.747126	-0.208517	1023.7308	1032.7939	1066.5931
	C	4.608734	0.316401	0.211226	1110.9464	1157.5953	1162.5774
	C	5.240073	-0.868143	-0.057523	1172.6617	1181.5282	1184.4721
C	4.487578	-2.018714	-0.419321	1195.7494	1214.9688	1229.5257	
C	3.121972	-1.958144	-0.495657	1236.1369	1257.3734	1285.8937	
H	-0.685305	-1.953565	0.959480	1292.3920	1313.3222	1355.1715	

	H	-5.359854	-1.229195	-0.470121	1356.2081	1375.4826	1383.2547
	H	-4.959072	1.137679	-0.735392	1401.8485	1418.7510	1445.9489
	H	-2.264370	-3.795906	1.010085	1449.5014	1454.7880	1480.3869
	H	-4.608826	-3.482230	0.223032	1509.3505	1523.3177	1542.1899
	H	-3.462390	3.085315	-0.502605	1577.7889	1592.5582	1630.2171
	H	-1.351957	4.048305	0.020898	1631.6180	1648.5258	1666.1383
	H	1.061045	3.862330	0.473538	1669.9438	3155.5381	3157.5487
	H	3.065799	2.528288	0.527369	3158.0321	3159.6895	3161.3174
	H	0.488877	-1.548168	-0.573226	3162.4522	3169.8863	3175.4777
	H	5.181597	1.198286	0.478488	3177.3386	3179.6283	3186.7293
	H	6.320702	-0.934618	-0.000123	3188.0587	3206.8841	3227.7721
	H	5.004162	-2.947341	-0.634262			
	H	2.546905	-2.836726	-0.769197			
p3	C	1.883055	0.823439	0.114438			
	C	3.226195	1.119416	-0.281569	34.2210	58.9351	72.9700
	C	1.137082	1.886889	0.686304	87.6128	95.1859	123.6356
	C	1.400255	-0.544167	0.007605	159.8853	182.5966	223.0483
	C	3.697605	2.452121	-0.237598	239.8714	271.6815	280.7827
	C	4.107829	0.058193	-0.645376	321.7176	368.6573	387.8235
	C	1.633337	3.171998	0.750547	418.4649	433.1447	443.7842
	C	2.357893	-1.565879	-0.202427	465.7746	482.8817	502.7307
	C	2.912633	3.471025	0.250361	533.3691	537.0881	548.5204
	C	3.705001	-1.234928	-0.544790	584.9433	594.7804	618.3368
	C	0.003635	-0.940594	0.099897	625.1897	639.1427	680.5553
	C	1.990573	-2.939242	-0.074761	690.9512	702.1133	709.3740
	C	-0.316537	-2.323229	0.273868	757.2983	759.3506	767.3005
	C	0.713174	-3.303736	0.218146	799.1317	810.0333	823.5906
	C	-1.671209	-2.710718	0.425359	835.9799	837.0513	858.0817
	C	-2.694073	-1.804870	0.331000	864.2081	885.5454	907.8414
	C	-1.084102	-0.052268	-0.075544	930.3049	962.7725	967.8969
	C	-2.413880	-0.446375	0.031856	976.2796	982.7919	986.9824
	C	-3.455881	0.552691	-0.188291	991.0396	1005.3082	1024.1963
	C	-4.789705	0.365504	-0.114315	1046.7609	1067.9368	1127.2259
	C	-5.740403	1.391203	-0.338170	1160.2924	1173.3196	1183.2360
	C	-6.576681	2.240514	-0.522448	1185.4423	1207.0348	1228.7785
	H	0.177351	1.683893	1.136646	1237.2671	1244.9503	1260.1477
	H	4.710666	2.651696	-0.570956	1283.2203	1298.6134	1327.4182
	H	5.120781	0.302667	-0.946617	1338.1562	1353.6331	1371.9774
	H	1.036644	3.952221	1.209549	1388.2759	1398.3051	1427.4274
	H	3.289891	4.486518	0.287444	1450.9155	1460.3767	1478.9067
	H	4.396373	-2.046019	-0.746761	1523.9276	1539.5608	1555.4915
H	2.764321	-3.689946	-0.194681	1588.5438	1631.8444	1647.5118	
H	0.450331	-4.347083	0.355234	1648.8585	1660.0829	1665.8374	
H	-1.889559	-3.760124	0.593726	2193.9386	3143.1189	3153.1082	
H	-3.717526	-2.140025	0.446051	3157.6751	3159.4312	3160.8849	
H	-0.888950	0.970854	-0.360843	3162.9383	3170.4807	3177.0890	
H	-3.101657	1.549742	-0.435002	3179.4186	3186.6518	3189.2934	
H	-5.197746	-0.611447	0.128783	3208.0229	3227.5907	3477.3975	
H	-7.305703	2.995123	-0.687109				
p4	C	1.836855	0.866758	0.122146	32.7038	41.6295	50.4328
	C	3.156599	1.249183	-0.279276	81.2916	94.9054	117.3656
	C	1.029288	1.877641	0.705963	163.0249	165.6755	202.3204
	C	1.440212	-0.527430	0.006746	254.2740	270.0613	288.7863
	C	3.544537	2.608356	-0.227129	319.7626	336.6531	379.4466
	C	4.100091	0.248458	-0.657829	411.5020	427.3791	446.8301
	C	1.445208	3.190427	0.777553	470.3864	479.8347	500.5515
	C	2.457777	-1.485007	-0.218915	530.3527	538.7429	549.9852
	C	2.700660	3.572473	0.273253	584.8964	589.6175	627.6339
	C	3.779095	-1.068196	-0.566765	636.3897	656.7103	692.0329
	C	0.070690	-1.011649	0.106003	694.2149	707.2942	710.3998
	C	2.178261	-2.880454	-0.099929	757.8468	766.0782	782.6100
	C	-0.161252	-2.414667	0.271743	802.7445	810.2055	831.0021
	C	0.929701	-3.327120	0.199761	840.3536	862.1535	874.0158
	C	-1.484354	-2.892673	0.429383	885.0827	932.6774	939.1181
	C	-2.565346	-2.053465	0.351408	951.7603	965.2207	971.0492
	C	-1.067178	-0.188261	-0.054234	978.3793	983.6489	993.6796
	C	-2.365514	-0.677865	0.064696	1006.5149	1006.6973	1036.0997
	C	-3.480481	0.184869	-0.118580	1067.5212	1102.2686	1129.3007
	C	-4.443838	0.904240	-0.268748	1159.9314	1173.1063	1179.9330
C	-5.539549	1.782827	-0.455221	1184.9402	1210.0284	1230.8885	

	C	-6.829031	1.434772	-0.348660	1237.8130	1250.4063	1273.5334
	H	0.085639	1.613350	1.158268	1291.6090	1319.3802	1326.9018
	H	4.541167	2.873060	-0.564672	1346.3404	1365.1755	1385.7829
	H	5.093812	0.558191	-0.963113	1396.1492	1420.3153	1445.6220
	H	0.803126	3.928438	1.244993	1451.4311	1462.6736	1476.1608
	H	3.014098	4.609231	0.316386	1518.5337	1538.7670	1550.4424
	H	4.518147	-1.832932	-0.780420	1585.9514	1630.0180	1644.5238
	H	2.997027	-3.579729	-0.231439	1647.7591	1663.7513	1665.9243
	H	0.734460	-4.385997	0.330423	2294.1481	3129.3622	3146.0635
	H	-1.632960	-3.955656	0.587428	3157.5280	3159.4054	3160.9427
	H	-3.574007	-2.430832	0.464676	3164.6881	3170.6045	3177.0317
	H	-0.948269	0.847322	-0.330725	3179.4161	3186.5586	3194.7235
	H	-5.285996	2.811355	-0.702505	3217.9769	3235.5237	3238.2050
	H	-7.125699	0.421755	-0.104340			
	H	-7.615099	2.163156	-0.505180			
	C	2.181969	-0.663056	-0.081437			
	C	3.561744	-0.703996	0.296235	-105.0790	12.0728	24.5419
	C	1.623986	-1.864897	-0.589710	30.4544	61.7739	81.4489
	C	1.469767	0.604301	-0.022151	86.7955	132.1877	165.3175
	C	4.257198	-1.935628	0.298213	188.4489	214.8102	228.5510
	C	4.250456	0.509215	0.595056	260.8715	280.9923	325.8026
	C	2.335358	-3.046409	-0.610734	360.7621	378.7928	411.9825
	C	2.237606	1.784785	0.125709	438.5878	440.9086	477.3040
	C	3.654561	-3.096508	-0.127875	513.4730	518.2067	526.4785
	C	3.626627	1.707069	0.450538	547.4696	558.7732	577.3347
	C	0.025779	0.746139	-0.101214	593.2052	625.7803	630.3823
	C	1.634330	3.067430	-0.046517	674.4013	677.4068	686.4500
	C	-0.540391	2.044826	-0.316483	703.1227	717.8997	749.1750
	C	0.309525	3.190811	-0.320797	754.7510	760.0701	782.2078
	C	-1.941489	2.206337	-0.447796	805.5357	824.9241	829.1555
	C	-2.808664	1.139038	-0.311994	842.8189	855.6981	877.9572
	C	-0.895152	-0.322477	0.127877	894.6640	896.7851	917.9142
	C	-2.227974	-0.081232	0.003494	958.0370	959.1133	966.9252
	C	-3.965464	-1.960005	0.545977	975.0852	982.4510	984.2681
	C	-5.056712	-1.711720	-0.206661	1000.9222	1012.4940	1057.4619
	C	-6.132060	-0.881173	0.196211	1077.8095	1112.7003	1123.5676
	C	-7.061933	-0.178496	0.507948	1147.4810	1171.0142	1175.1239
	H	0.636839	-1.851820	-1.025820	1183.7256	1205.5656	1223.8430
	H	5.294432	-1.941060	0.616754	1235.4113	1245.9022	1266.1166
	H	5.295013	0.457976	0.883067	1305.4496	1309.6385	1345.4621
	H	1.876613	-3.938439	-1.022437	1352.0497	1369.1097	1394.8037
	H	4.202207	-4.031960	-0.130225	1409.6505	1435.6794	1440.6885
	H	4.169195	2.633879	0.603599	1451.6548	1471.7630	1501.7910
	H	2.267079	3.945535	0.025260	1529.9233	1545.9937	1589.2275
	H	-0.133198	4.166415	-0.490291	1604.0112	1612.5906	1635.7065
	H	-2.330905	3.202183	-0.637045	1647.7344	1665.1571	2183.6016
	H	-3.881186	1.258921	-0.412838	3140.7042	3151.8414	3156.0524
	H	-0.536850	-1.288089	0.455196	3157.0480	3159.0807	3160.6037
	H	-3.202671	-2.644358	0.198945	3169.2096	3176.4002	3178.7545
	H	-3.881278	-1.589291	1.559199	3179.9491	3185.9154	3196.4620
	H	-5.130695	-2.142687	-1.201658	3226.1540	3248.8228	3475.8164
	H	-7.878993	0.436667	0.794946			
	C	1.871112	-0.748707	-0.186757	-196.8272	5.3687	16.6543
	C	3.112121	-1.109440	0.428363	38.0772	51.6232	77.6764
	C	1.271178	-1.720545	-1.029264	80.1097	105.7963	133.4034
	C	1.354719	0.599017	-0.001030	182.1413	214.1682	230.4630
	C	3.604593	-2.429615	0.304821	260.3498	279.8177	321.7791
	C	3.885051	-0.116048	1.099930	331.6059	378.7735	412.4255
	C	1.790980	-2.991276	-1.160922	437.2512	441.1943	477.0330
	C	2.232787	1.572049	0.535011	506.3166	514.2512	526.3402
	C	2.949877	-3.367180	-0.459757	543.8369	561.3814	577.7224
	C	3.488243	1.182918	1.094675	593.8013	626.1638	643.2340
	C	0.001218	1.018392	-0.325226	669.6461	675.5987	688.9031
	C	1.875780	2.954595	0.524142	695.3558	704.6005	752.4695
	C	-0.306901	2.417509	-0.367507	757.6847	759.9079	779.3383
	C	0.678506	3.368203	0.033372	806.7105	824.6132	827.8666
	C	-1.603942	2.857070	-0.728063	847.3777	854.7675	880.7395
	C	-2.623084	1.961262	-0.989317	898.2709	901.2808	940.0497
	C	-1.092143	0.117904	-0.507533	952.4492	954.7363	965.8138
	C	-2.314752	0.614675	-0.840386	974.1874	981.7906	1001.0183

	C	-4.162516	-1.062270	-1.139077	1001.1760	1012.2661	1056.3505
	C	-4.517380	-1.452604	-0.045155	1076.1058	1111.6994	1123.0162
	C	-4.838779	-1.875984	1.265284	1147.0775	1170.7845	1174.8593
	C	-5.753672	-1.290889	2.052318	1183.6509	1205.6828	1224.0540
	H	0.415170	-1.451619	-1.628729	1235.3688	1246.1927	1265.5678
	H	4.533645	-2.681752	0.805534	1309.2678	1316.0491	1345.5828
	H	4.820898	-0.409336	1.563528	1352.7355	1368.7700	1394.7045
	H	1.308948	-3.698324	-1.826771	1408.7938	1440.2589	1441.0235
	H	3.343342	-4.372906	-0.553484	1451.6427	1471.6056	1500.5427
	H	4.110837	1.951990	1.539397	1529.8704	1545.4963	1589.1436
	H	2.596792	3.673308	0.898658	1609.7150	1635.6403	1642.4637
	H	0.431046	4.423519	-0.008465	1647.8521	1665.3851	2116.9811
	H	-1.793437	3.925539	-0.771633	3134.8333	3147.7470	3149.0881
	H	-3.615667	2.301047	-1.263092	3156.3284	3158.3195	3159.8296
	H	-0.966927	-0.939577	-0.325253	3169.1935	3172.9960	3175.8307
	H	-4.041611	-0.879519	-2.179012	3178.2688	3185.5699	3201.8407
	H	-4.291603	-2.740944	1.632614	3228.7270	3238.1570	3458.7711
	H	-6.317619	-0.427151	1.721413			
	H	-5.951794	-1.668490	3.047752			
TS [i3]-p3	C	1.628273	-0.917681	-0.135347	-549.4400	31.8828	55.9790
	C	2.906009	-1.429275	0.257540	60.3551	83.7511	90.7434
	C	0.722250	-1.841852	-0.719005	124.8739	150.5741	176.8923
	C	1.371284	0.507629	-0.014518	204.8063	234.1915	267.7564
	C	3.156535	-2.820387	0.201625	285.4775	313.3143	315.0433
	C	3.945524	-0.526468	0.630278	352.6183	362.0083	388.7325
	C	1.005705	-3.189139	-0.795929	414.5372	433.8347	452.4023
	C	2.478975	1.360772	0.202158	470.9277	475.0489	496.5573
	C	2.218915	-3.694898	-0.296351	533.0458	536.8443	548.4063
	C	3.755121	0.815785	0.540504	576.7657	588.0589	620.0504
	C	0.053929	1.121851	-0.101558	626.6111	639.2966	679.3091
	C	2.335648	2.777327	0.082184	692.3889	697.9533	709.7212
	C	-0.041253	2.540579	-0.270455	753.6676	758.7729	767.1883
	C	1.134555	3.342775	-0.209846	798.9971	810.0963	823.1339
	C	-1.313879	3.139476	-0.411734	836.4393	842.9978	852.9396
	C	-2.465215	2.399186	-0.315836	866.4732	885.1299	916.0330
	C	-1.154761	0.412295	0.076943	929.1621	964.2181	968.8936
	C	-2.403150	1.013524	-0.032124	977.1653	983.3704	990.0166
	C	-3.663275	0.281418	0.149338	991.2661	1005.7940	1036.7574
	C	-3.813754	-1.069646	0.213330	1043.6177	1068.8388	1126.5989
	C	-5.066275	-1.713108	0.303342	1161.9328	1173.1278	1180.3269
	C	-6.122232	-2.292701	0.379604	1185.0870	1199.0683	1213.5585
	H	-0.189844	-1.481302	-1.170457	1232.8729	1238.9521	1256.2879
	H	4.123473	-3.183623	0.533777	1282.0784	1302.6590	1313.4415
	H	4.905873	-0.932421	0.929430	1332.4068	1353.9378	1370.1898
	H	0.293881	-3.858828	-1.265333	1386.9456	1398.1036	1430.3723
	H	2.427790	-4.757482	-0.342845	1450.8152	1462.0983	1474.6596
	H	4.567621	1.503701	0.748506	1522.8623	1538.1648	1552.6044
	H	3.219647	3.393677	0.205852	1589.0144	1608.3666	1634.6210
	H	1.042275	4.415372	-0.341872	1647.3732	1649.9767	1664.5566
	H	-1.366906	4.211697	-0.568046	2180.8622	3145.9502	3157.7784
	H	-3.432732	2.879048	-0.415712	3158.4951	3159.8389	3161.0498
	H	-1.105954	-0.624547	0.370972	3162.0943	3170.2643	3176.8550
H	-3.934055	0.763543	2.175716	3178.1489	3179.9637	3186.7386	
H	-4.565755	0.879689	0.072014	3212.3057	3230.6544	3476.2423	
H	-2.942982	-1.718800	0.215290				
H	-7.055918	-2.794511	0.447859				
TS [i3]-[i8]	C	-1.426916	0.737638	-0.097604	-1725.4322	28.1825	61.1102
	C	-2.769852	1.152276	0.171102	65.9332	75.5570	123.5347
	C	-0.507811	1.747655	-0.473950	144.8305	169.5902	210.3276
	C	-1.097637	-0.677334	-0.044945	217.4429	251.9788	269.3580
	C	-3.096148	2.528419	0.173818	297.5547	350.2327	379.0390
	C	-3.785992	0.173381	0.379857	399.4588	416.9502	437.6258
	C	-0.856741	3.081823	-0.487696	458.3068	469.5907	486.3615
	C	-2.164003	-1.603691	0.048804	525.5088	529.1091	534.7779
	C	-2.155824	3.484739	-0.132716	540.8118	564.5802	588.7077
	C	-3.500215	-1.149741	0.271661	606.0610	618.6601	645.2150
	C	0.254929	-1.207023	-0.072845	665.3312	681.0389	691.0470
	C	-1.924351	-3.005958	-0.072895	720.5167	744.6680	752.5442
	C	0.458085	-2.624334	-0.223969	764.1781	789.4582	807.8406
	C	-0.669858	-3.495572	-0.250698	813.8824	834.0892	848.0397

	C	1.769077	-3.158924	-0.286144	856.0469	859.8029	885.6221	
	C	2.888093	-2.370444	-0.142889	899.8599	947.6878	958.5524	
	C	1.443030	-0.478430	0.110894	966.5212	972.6494	982.0077	
	C	2.716164	-0.992831	0.096291	984.2195	1001.6939	1020.4141	
	C	3.798190	0.030861	0.373047	1051.0064	1067.1179	1076.0360	
	C	3.040673	1.298334	0.823045	1117.1437	1155.3611	1171.7496	
	C	3.308368	2.527283	0.155160	1177.3813	1183.7885	1185.9478	
	C	3.505339	3.561293	-0.437395	1205.2119	1211.1132	1235.1543	
	H	0.482096	1.470988	-0.800160	1239.5285	1250.0848	1285.0926	
	H	-4.117149	2.815609	0.403014	1286.3826	1309.4841	1343.8035	
	H	-4.797581	0.507884	0.583953	1356.4828	1360.7779	1374.5163	
	H	-0.121163	3.819355	-0.787106	1395.5210	1406.7479	1443.6917	
	H	-2.420552	4.536029	-0.131971	1453.5797	1469.1780	1484.7205	
	H	-4.283109	-1.893658	0.373590	1521.0157	1528.9806	1548.9397	
	H	-2.776544	-3.676002	-0.034855	1581.6243	1630.7417	1640.2833	
	H	-0.501292	-4.560523	-0.371127	1648.3730	1666.5307	1690.4042	
	H	1.874647	-4.229876	-0.423974	2162.2014	3034.5675	3065.0208	
	H	3.880918	-2.807691	-0.178303	3088.5470	3153.6727	3156.1016	
	H	1.870101	0.856195	0.518831	3157.7249	3159.5491	3172.2804	
	H	4.500675	-0.310420	1.139629	3173.1059	3175.6248	3178.0979	
	H	4.382826	0.235036	-0.528729	3187.1973	3233.4097	3474.6891	
	H	2.971454	1.407970	1.906628				
	H	3.695073	4.472596	-0.949022				
	C	2.111099	-0.665392	-0.093379				
	C	3.512477	-0.663853	0.197960	-1652.4587		28.8689	61.9177
	C	1.551986	-1.896158	-0.526331	76.4736	79.1970	128.0825	
	C	1.374216	0.588000	-0.034254	133.9881	167.5335	203.8869	
	C	4.234662	-1.880152	0.200530	232.9040	259.3802	271.5706	
	C	4.190989	0.573483	0.406975	309.9299	315.1038	382.8927	
	C	2.287584	-3.062450	-0.550900	398.9959	408.1611	426.6440	
	C	2.124507	1.787303	0.013171	442.5303	471.3278	492.9776	
	C	3.634214	-3.067835	-0.147285	519.5037	528.2128	538.8241	
	C	3.532402	1.751338	0.252978	543.7338	589.2467	593.5605	
	C	-0.077548	0.694361	-0.021460	603.9617	623.2475	641.2616	
	C	1.484544	3.049214	-0.178510	668.0920	678.2021	704.4087	
	C	-0.678127	1.974730	-0.265616	709.7328	749.9179	757.0401	
	C	0.143410	3.134823	-0.377845	763.0297	800.1808	804.7909	
	C	-2.094283	2.104101	-0.308129	808.6284	825.9344	844.8673	
	C	-2.849092	1.001194	-0.050341	846.1221	879.0684	884.6252	
	C	-0.938498	-0.384069	0.321540	898.3021	917.9376	950.4162	
	C	-2.311197	-0.238658	0.305555	965.3629	972.5151	980.4506	
	C	-3.367748	-1.272668	0.644133	982.3577	1001.7456	1023.8378	
	C	-5.820869	-0.995306	-0.013407	1026.1678	1067.2869	1074.7163	
	C	-6.763979	-1.399656	-0.649156	1123.9211	1165.1733	1169.9911	
	C	-4.698741	-0.490041	0.706286	1179.6445	1187.4486	1190.8442	
	H	0.540229	-1.918838	-0.901699	1203.0210	1227.6198	1232.0749	
	H	5.289276	-1.852397	0.454251	1243.4262	1259.7002	1273.3236	
	H	5.252125	0.554901	0.631191	1297.5010	1310.8062	1341.5900	
	H	1.825733	-3.977569	-0.904284	1361.5549	1365.3909	1374.7363	
	H	4.202115	-3.991140	-0.150990	1398.0429	1404.5607	1439.6900	
	H	4.062137	2.694576	0.333486	1452.3826	1469.7504	1481.1113	
	H	2.101326	3.941590	-0.185775	1508.6940	1530.4308	1548.3428	
	H	-0.330795	4.092076	-0.565667	1589.6560	1623.5858	1638.1928	
	H	-2.529191	3.077497	-0.511382	1647.6406	1662.4677	1664.7099	
	H	-0.514730	-1.319024	0.660185	2168.3478	3038.1704	3067.2864	
	H	-3.419704	-2.040943	-0.132482	3083.9182	3156.2794	3157.3989	
	H	-3.160778	-1.783938	1.588878	3159.0840	3160.5709	3169.3480	
	H	-7.595687	-1.760983	-1.202245	3176.3031	3178.5476	3185.8508	
	H	-4.255966	0.589594	0.177469	3198.3513	3224.8503	3475.3519	
	H	-4.958138	-0.159254	1.713976				
	C	-1.655394	0.946775	-0.136124	-613.9326	27.1555	36.8705	
	C	-2.925271	1.485840	0.245669	54.2620	79.9883	97.0150	
	C	-0.725658	1.850786	-0.713274	103.9500	118.6694	163.9560	
	C	-1.429258	-0.484115	-0.009562	178.0949	205.9814	256.4966	
	C	-3.147699	2.881233	0.182769	261.3933	281.1830	320.8393	
	C	-3.986233	0.606677	0.615147	342.2735	377.9927	402.3888	
	C	-0.981166	3.203368	-0.795942	420.5235	443.4303	445.6682	
	C	-2.556634	-1.312494	0.205699	479.3098	491.2943	510.7717	
	C	-2.188502	3.735091	-0.310127	535.5808	538.1142	554.9654	
	C	-3.823336	-0.739331	0.533618	570.9438	587.3245	629.6624	

	C	-0.126645	-1.128592	-0.088108	639.9399	653.8993	690.1093
	C	-2.443496	-2.731851	0.096217	694.1183	707.7075	712.8329
	C	-0.060508	-2.549633	-0.244683	758.1089	766.4201	784.3139
	C	-1.253169	-3.325673	-0.184170	802.9791	810.4516	831.4971
	C	1.198595	-3.182303	-0.380262	840.4563	862.0788	875.3314
	C	2.370472	-2.477025	-0.288441	885.4310	934.2641	937.6248
	C	1.099793	-0.445059	0.084820	952.4928	965.6225	971.7011
	C	2.329106	-1.086877	-0.016947	978.7283	984.2088	994.0995
	C	3.536917	-0.338106	0.158172	1000.3083	1006.4390	1035.6847
	C	4.445017	0.475081	0.092606	1067.0556	1103.0787	1129.5124
	C	5.567666	1.329554	0.075197	1160.2945	1173.1324	1180.4369
	C	5.596809	2.564482	0.601030	1184.9280	1209.8078	1230.7794
	H	0.185411	1.473428	-1.152005	1237.6540	1249.4997	1270.4789
	H	-4.109939	3.264715	0.505710	1287.3319	1315.5264	1326.3889
	H	-4.939876	1.034244	0.905559	1346.9734	1365.3221	1385.2376
	H	-0.249907	3.856902	-1.258107	1396.1200	1420.6441	1444.2938
	H	-2.375637	4.801523	-0.361838	1451.2741	1460.7611	1475.9769
	H	-4.651039	-1.409354	0.740058	1519.9560	1538.1457	1551.3560
	H	-3.341317	-3.328042	0.219245	1586.5760	1630.3980	1640.3135
	H	-1.183511	-4.400970	-0.307510	1647.7293	1650.1043	1664.3852
	H	1.222472	-4.256489	-0.529831	2218.0057	3130.6599	3147.3108
	H	3.328434	-2.973434	-0.377785	3157.7332	3159.6291	3161.1985
	H	1.101512	0.598683	0.355751	3165.8933	3170.5576	3177.2794
	H	4.281002	-1.425068	1.689760	3179.6575	3186.5576	3197.0897
	H	6.458265	0.935802	-0.409598	3218.1082	3238.1103	3238.9064
	H	4.731779	2.992427	1.093205			
	H	6.493915	3.168674	0.547571			
	C	1.573450	-0.413971	-0.193688	-458.9975	55.7825	58.0577
	C	2.971279	-0.434548	0.112320	74.7196	105.5829	119.2246
	C	1.017174	-1.589500	-0.756139	151.5376	181.7647	209.1575
	C	0.823624	0.816639	-0.011914	247.3130	264.5522	298.4216
	C	3.706961	-1.632901	-0.041031	326.0742	339.6059	371.8065
	C	3.626468	0.769675	0.506204	393.9201	430.0377	438.5088
	C	1.764812	-2.735308	-0.925888	451.0851	473.9199	491.8052
	C	1.553064	2.006208	0.227051	523.0117	528.2767	535.8380
	C	3.116952	-2.771072	-0.540819	573.8679	586.4356	603.6050
	C	2.951874	1.949159	0.511913	634.4808	670.1354	676.7104
	C	-0.623937	0.915123	-0.103221	680.4770	701.7174	723.5590
	C	0.907472	3.278201	0.161065	748.7975	762.7195	769.7439
	C	-1.220637	2.211976	-0.260624	781.3171	799.2947	812.7634
	C	-0.414093	3.380877	-0.139399	827.9694	835.4240	851.8183
	C	-2.613846	2.312748	-0.479823	861.6981	882.7619	885.6787
	C	-3.422541	1.202904	-0.465301	944.3683	955.4747	963.6518
	C	-1.530760	-0.156104	0.012117	969.1224	976.2348	979.9466
	C	-2.891065	-0.077023	-0.156896	995.1663	1008.7564	1025.1730
	C	-3.878846	-1.215747	0.059094	1049.0401	1066.3697	1114.3776
	C	-2.109449	-2.588300	1.041939	1156.7436	1167.2468	1177.4381
	C	-1.137273	-1.932763	1.399260	1182.5499	1184.3675	1200.8449
	C	-3.281782	-2.635501	0.167601	1209.6841	1228.0996	1238.7194
	H	-0.014688	-1.580055	-1.073983	1243.5045	1258.7901	1295.5432
	H	4.760380	-1.629178	0.219277	1333.5330	1341.5284	1358.6470
	H	4.683537	0.733645	0.747462	1361.9672	1378.8609	1391.6038
	H	1.305429	-3.612746	-1.366782	1398.5677	1442.1107	1452.2696
	H	3.694889	-3.680092	-0.663735	1465.3718	1471.3615	1480.1462
	H	3.465384	2.876725	0.741973	1505.7776	1529.5022	1543.9972
	H	1.508513	4.167532	0.317930	1576.2285	1626.7880	1641.7599
	H	-0.886034	4.351988	-0.246846	1647.7779	1663.8437	2024.9316
	H	-3.042415	3.296152	-0.641398	3012.6497	3019.8741	3049.5809
	H	-4.490550	1.306619	-0.634868	3059.3129	3144.1633	3155.0672
	H	-4.437398	-1.003482	0.978633	3156.6861	3158.5372	3169.6093
	H	-4.613500	-1.208100	-0.753055	3170.3799	3174.5621	3177.0791
	H	-0.249714	-1.658458	1.921779	3184.6513	3214.7024	3424.6886
	H	-2.970489	-2.996797	-0.819540			
	H	-4.046749	-3.328385	0.530223			
TS [i8]-[i10]							
	C	-1.627959	-0.413816	-0.221800	-453.0873	54.1396	63.8185
	C	-3.014620	-0.403204	0.133163	91.2977	103.5367	126.9684
	C	-1.127424	-1.590294	-0.835290	145.6392	182.7965	206.5150
	C	-0.835351	0.787397	-0.024912	263.8186	271.6841	290.8217
	C	-3.792187	-1.573426	-0.032844	340.9449	358.0244	367.4698
	C	-3.616802	0.803276	0.597210	400.5113	428.6298	442.0749
TS [i8]-[i9]							

	C	-1.914881	-2.707994	-1.011505	460.1486	477.0993	495.0545
	C	-1.514652	1.985161	0.300287	517.2415	533.6358	537.2911
	C	-3.255391	-2.713421	-0.584918	561.5967	598.2082	626.9897
	C	-2.903240	1.959342	0.632827	631.5115	670.8529	681.1935
	C	0.607811	0.847561	-0.185186	694.9220	700.8823	721.5709
	C	-0.827099	3.237613	0.275718	750.1422	763.7010	778.9777
	C	1.247602	2.130637	-0.292883	791.9456	792.9746	812.6633
	C	0.485145	3.315105	-0.067752	828.8454	834.9453	855.4713
	C	2.632053	2.200705	-0.564087	864.2486	879.5700	883.9603
	C	3.400169	1.063238	-0.671721	933.5320	951.0386	964.3947
	C	1.475894	-0.256265	-0.196786	970.2848	975.4075	980.9281
	C	2.828620	-0.211587	-0.449933	987.0862	996.8108	1018.0597
	C	3.682104	-1.458607	-0.436975	1049.7708	1066.5145	1115.9848
	C	2.317093	-2.292074	1.413350	1154.4907	1168.2707	1173.5113
	C	1.159502	-1.890574	1.324199	1180.3668	1184.0661	1201.0533
	C	3.695044	-2.172826	0.953634	1210.5314	1219.8311	1238.7859
	H	-0.104392	-1.605215	-1.183730	1243.1711	1262.6869	1297.5031
	H	-4.835480	-1.546079	0.264170	1315.0714	1337.1497	1355.9336
	H	-4.665706	0.789824	0.873677	1361.2486	1373.7315	1393.0750
	H	-1.497147	-3.585550	-1.491954	1398.8044	1437.7509	1452.1135
	H	-3.865372	-3.600147	-0.715194	1465.7253	1477.2132	1489.1016
	H	-3.377564	2.890691	0.923639	1510.3112	1526.5924	1544.8900
	H	-1.390924	4.136001	0.503326	1575.8494	1625.2193	1637.0467
	H	0.985370	4.275532	-0.135936	1647.6031	1664.3242	2015.0031
	H	3.089884	3.178358	-0.669646	3027.9998	3035.8869	3063.1516
	H	4.461150	1.139823	-0.890306	3082.5999	3148.3894	3155.3214
	H	3.300163	-2.176245	-1.168705	3157.0620	3158.9341	3169.3005
	H	4.709090	-1.215047	-0.721178	3171.8393	3174.9295	3177.3013
	H	0.121282	-1.820538	1.556843	3184.3699	3200.2502	3414.6790
	H	4.276518	-1.590858	1.677040			
	H	4.184542	-3.146229	0.855192			
	C	2.074511	-0.495007	-0.109079			
	C	3.427537	-0.337137	0.330458	-369.2873	42.1225	56.7181
	C	1.733711	-1.747124	-0.684294	82.0840	104.8340	115.0446
	C	1.170092	0.643075	-0.042227	152.5775	176.0198	226.3611
	C	4.305364	-1.446386	0.325577	238.1245	279.1822	296.9088
	C	3.907052	0.955596	0.697005	323.9820	343.2785	379.4457
	C	2.620514	-2.803021	-0.711041	396.4277	418.3597	437.3748
	C	1.741309	1.921310	0.169584	456.0620	475.9755	482.3495
	C	3.909680	-2.668434	-0.166668	524.8970	528.2761	540.6251
	C	3.111032	2.047020	0.555900	568.3555	591.7184	625.5858
	C	-0.275926	0.563056	-0.180864	638.0380	657.2385	669.6506
	C	0.955562	3.101268	0.001163	692.8342	708.1247	718.1252
	C	-1.018191	1.767254	-0.393581	739.5495	757.1101	761.9141
	C	-0.359958	3.029721	-0.333201	792.4136	799.8169	809.1017
	C	-2.427081	1.699685	-0.576126	828.7308	844.3148	854.3858
	C	-3.051845	0.495243	-0.491258	871.3152	873.6553	882.9993
	C	-1.018907	-0.636448	-0.013144	919.4296	934.2929	964.1430
	C	-2.396659	-0.699210	-0.161492	966.7699	974.9411	980.8272
	C	-3.144594	-2.005504	0.010734	993.2133	1002.1818	1020.2263
	C	-5.192606	-0.788124	0.580359	1033.8784	1067.1765	1125.6542
	C	-5.344206	0.285570	0.020335	1164.8423	1169.8552	1181.5314
	C	-4.356444	-1.916016	0.980744	1190.2998	1195.2947	1202.0312
	H	0.775736	-1.867864	-1.166748	1217.5189	1231.0635	1235.3631
	H	5.316660	-1.304320	0.692375	1246.4622	1272.4873	1308.4209
	H	4.934004	1.055439	1.031741	1326.1203	1336.9780	1354.5170
	H	2.324726	-3.737314	-1.175110	1369.0763	1374.3897	1396.2706
	H	4.596332	-3.507227	-0.173807	1402.3640	1438.5367	1452.3125
	H	3.496154	3.040746	0.758778	1464.8334	1476.4240	1481.4905
	H	1.441987	4.063212	0.123944	1499.7794	1529.4164	1545.2933
	H	-0.941300	3.930138	-0.500507	1583.8923	1613.2237	1636.7434
	H	-2.974410	2.621956	-0.749026	1647.4840	1663.2668	2068.1156
	H	-0.504800	-1.536325	0.294152	3023.5989	3027.8260	3060.8288
	H	-3.524777	-2.329099	-0.964387	3075.7503	3142.6556	3155.8529
	H	-2.460535	-2.781214	0.364936	3157.7002	3159.3969	3168.3791
	H	-5.777125	1.180484	-0.361839	3175.2614	3177.5793	3185.0619
	H	-4.011754	-1.767471	2.009955	3196.0947	3224.8920	3435.4817
	H	-4.910578	-2.859454	0.962247			
TS [i5]-[i6]	C	-1.590804	-0.375001	-0.176477	-1663.9030	61.5241	71.2085
TS [i9]-[i11]	C	-2.968720	-0.333824	0.203244	85.8868	114.5769	127.0480

	C	-1.142672	-1.531645	-0.862179	174.0576	197.8934	239.4679
	C	-0.757821	0.798651	0.031975	261.2728	297.4943	311.9123
	C	-3.779687	-1.480230	0.030267	344.1862	393.0600	417.6840
	C	-3.535899	0.891001	0.664529	440.4403	454.6591	459.2317
	C	-1.965096	-2.619878	-1.056790	487.7157	496.7520	503.6751
	C	-1.423380	2.026707	0.273636	539.7350	543.7924	560.1709
	C	-3.287168	-2.612858	-0.575784	600.0806	609.6216	621.1664
	C	-2.805968	2.037471	0.632068	663.5665	669.0287	692.3149
	C	0.693148	0.821597	-0.067299	704.0380	733.7106	755.3709
	C	-0.729728	3.263858	0.115765	759.4066	766.2746	779.9052
	C	1.319450	2.073246	-0.362708	787.4462	804.7403	817.2769
	C	0.567889	3.284030	-0.286240	835.4873	850.6157	855.6518
	C	2.699982	2.118722	-0.653945	880.9552	895.3183	918.7591
	C	3.480435	0.989568	-0.550502	941.6703	954.1255	961.5508
	C	1.557078	-0.296382	0.222638	968.6022	978.1746	986.1681
	C	2.935676	-0.204395	-0.057722	994.4389	1048.0388	1059.9883
	C	3.881630	-1.339342	0.317984	1069.4383	1095.5956	1149.1076
	C	1.786518	-2.663227	0.733400	1169.8732	1174.0218	1182.2963
	C	1.120643	-1.479890	0.954306	1186.1272	1194.4386	1209.3682
	C	3.149298	-2.662899	0.372493	1212.6086	1229.8836	1236.7406
	H	-0.142328	-1.552941	-1.266270	1241.4594	1255.2288	1287.7402
	H	-4.814381	-1.435246	0.354022	1299.1144	1320.0786	1344.9340
	H	-4.577899	0.904045	0.966036	1358.3333	1371.7093	1385.6465
	H	-1.588469	-3.484522	-1.590992	1396.6705	1402.5037	1428.9372
	H	-3.921956	-3.480597	-0.715317	1447.9436	1450.7553	1468.1203
	H	-3.261323	2.989343	0.884304	1468.9343	1522.6723	1525.6936
	H	-1.279461	4.186924	0.265534	1550.7662	1579.0111	1608.0971
	H	1.073500	4.221465	-0.491479	1634.1945	1647.4543	1661.3758
	H	3.143155	3.068880	-0.931946	2099.6954	2974.3308	3045.2825
	H	4.542114	1.040557	-0.770149	3125.5902	3153.7628	3155.8392
	H	4.711029	-1.392559	-0.394410	3157.9880	3159.5537	3171.6066
	H	4.340652	-1.113682	1.291732	3173.5930	3175.7974	3178.5753
	H	0.245188	-1.421561	1.588151	3183.6867	3185.9554	3228.9832
	H	2.717241	-3.217635	1.488785			
	H	3.584110	-3.544149	-0.093955			
	C	1.586896	-0.371715	-0.176133	-1520.7852	59.8379	70.1530
	C	2.965009	-0.328366	0.198989	84.3903	117.4559	128.2184
	C	1.137791	-1.532163	-0.855045	172.0656	200.9439	239.9249
	C	0.753362	0.803492	0.030580	261.8014	298.3876	313.2714
	C	3.775207	-1.476349	0.031333	345.8708	392.9239	417.3023
	C	3.533857	0.899295	0.652226	439.5639	449.5318	470.5443
	C	1.958887	-2.621964	-1.045615	478.8265	494.9822	516.6750
	C	1.420055	2.033572	0.264355	539.6806	543.4783	556.2510
	C	3.281409	-2.612923	-0.565795	596.8001	610.4077	616.9625
	C	2.804375	2.045681	0.616784	664.5130	673.2397	686.7246
	C	-0.695178	0.826008	-0.059804	705.5718	732.9019	752.1999
	C	0.723744	3.268526	0.110158	756.1877	768.9369	775.5196
	C	-1.325688	2.073522	-0.352060	786.7234	800.5728	815.9539
	C	-0.577845	3.286015	-0.281382	837.2030	848.6473	856.1283
	C	-2.707914	2.112361	-0.647432	881.1724	894.6058	934.4362
	C	-3.484224	0.978874	-0.553756	942.2981	953.4840	961.9263
	C	-1.557715	-0.301941	0.229395	965.7466	971.4221	979.0491
	C	-2.937792	-0.215060	-0.065886	994.8312	1042.0476	1060.8654
	C	-3.871981	-1.351340	0.313667	1065.1841	1095.4358	1149.1713
	C	-1.809454	-2.708036	0.897040	1169.6899	1174.3192	1182.3006
	C	-1.121166	-1.460555	0.962496	1188.1915	1193.7461	1209.1035
	C	-3.137477	-2.662125	0.442336	1226.0220	1231.9552	1239.3325
	H	0.138747	-1.550626	-1.264061	1243.4364	1258.4689	1287.1919
	H	4.810379	-1.429864	0.353128	1290.6607	1330.5159	1353.6932
	H	4.576643	0.913398	0.950720	1356.3671	1367.1781	1384.5811
	H	1.582212	-3.489362	-1.575233	1395.1540	1398.0944	1435.1678
	H	3.915134	-3.482123	-0.699970	1437.5237	1449.7841	1456.9251
	H	3.260688	2.998433	0.863639	1467.8940	1519.9434	1523.8437
	H	1.272558	4.192805	0.255385	1548.2991	1573.7121	1602.4145
	H	-1.086478	4.222203	-0.484536	1632.4147	1647.5059	1660.4441
	H	-3.153990	3.061168	-0.925252	2113.6210	2957.8831	3047.3122
	H	-4.545423	1.026935	-0.776065	3120.8683	3154.9942	3156.9589
	H	-4.334386	-1.122323	1.287492	3159.1991	3160.5890	3172.1822
	H	-4.696436	-1.424710	-0.402447	3174.5152	3176.6971	3179.3516
	H	-0.219444	-1.393332	1.558062	3180.1557	3186.7434	3220.2845

	H	-2.110016	-3.047357	-0.308121			
	H	-3.695136	-3.584093	0.288545			
TS [i6]-[i7]	C	2.038163	-0.520823	-0.092759			
	C	3.430185	-0.352200	0.193135	-1700.3862	54.8562	61.9964
	C	1.629281	-1.804272	-0.538315	87.1421	117.1408	143.8342
	C	1.153553	0.632887	-0.014467	171.3200	213.4596	234.4567
	C	4.294615	-1.471518	0.175989	269.9479	289.2562	322.2147
	C	3.953996	0.956152	0.416483	344.9542	384.0382	407.2432
	C	2.500727	-2.872913	-0.580753	421.9041	443.1758	470.2601
	C	1.752990	1.916168	0.050199	478.1695	497.2564	519.9332
	C	3.840475	-2.719247	-0.184491	536.9402	545.5283	568.5335
	C	3.155427	2.047454	0.283505	596.6366	602.8739	635.9964
	C	-0.294090	0.564510	0.003186	643.3923	689.6827	708.7508
	C	0.960156	3.092409	-0.110639	711.4726	727.0900	756.6752
	C	-1.053665	1.759183	-0.205815	761.1036	763.6709	791.9794
	C	-0.384044	3.015782	-0.295306	804.7791	807.1441	810.7425
	C	-2.460701	1.694891	-0.265930	829.2305	841.4296	848.5460
	C	-3.157010	0.516069	-0.041003	883.3176	898.2262	908.3934
	C	-1.032495	-0.610381	0.324322	935.7000	944.8722	964.7501
	C	-2.405631	-0.649767	0.319291	973.3536	980.6693	987.8097
	C	-3.170773	-1.880339	0.791455	1004.3042	1022.0691	1066.3096
	C	-5.131217	-0.825518	-0.379028	1073.5683	1110.2944	1155.6068
	C	-4.605499	0.411354	-0.089729	1172.1206	1172.9734	1181.8517
	C	-4.454899	-2.006607	-0.008811	1187.7134	1197.4616	1207.9407
	H	0.625164	-1.944079	-0.909013	1220.2810	1229.1005	1243.2871
	H	5.339711	-1.319252	0.424955	1251.2263	1283.8818	1285.7264
	H	5.010928	1.064180	0.635203	1297.3764	1321.0480	1352.4397
	H	2.151131	-3.833285	-0.942941	1358.4393	1372.6629	1386.3964
	H	4.516496	-3.566430	-0.203093	1401.2102	1421.7689	1441.0029
	H	3.567297	3.046708	0.377177	1450.4342	1458.9801	1467.8952
	H	1.462276	4.053995	-0.104035	1480.4958	1514.9361	1534.3701
	H	-0.974665	3.910795	-0.458719	1543.9015	1588.7499	1630.6153
H	-3.012315	2.605867	-0.477365	1632.8114	1646.9141	1663.3867	
H	-0.499930	-1.489976	0.656933	2086.1234	2985.8295	3069.6087	
H	-2.562354	-2.783786	0.704029	3129.5471	3155.2599	3156.7906	
H	-3.406153	-1.765316	1.858937	3158.6375	3160.1886	3162.3256	
H	-5.216579	1.303392	-0.005416	3168.6800	3176.1289	3178.3709	
H	-5.662328	-1.701827	0.451312	3185.3879	3199.8619	3224.7469	
H	-4.695951	-2.940625	-0.511079				
TS [i11]-p2	C	-1.599488	-0.391049	-0.189755	-614.2902	64.4063	71.8890
	C	-2.979403	-0.358040	0.177828	89.2386	119.7419	164.5903
	C	-1.147302	-1.531160	-0.900284	173.1696	225.3504	240.1634
	C	-0.766944	0.781455	0.051720	269.5898	279.7282	308.6706
	C	-3.790829	-1.498124	-0.033435	339.8386	347.5175	401.2336
	C	-3.552363	0.855159	0.666968	421.4001	430.8477	455.9443
	C	-1.969195	-2.612492	-1.132739	473.8253	484.0456	500.9000
	C	-1.439258	2.003821	0.316259	527.0485	537.7712	544.4935
	C	-3.296466	-2.615416	-0.665328	557.0089	576.5925	613.6277
	C	-2.825178	2.002161	0.667891	634.8206	658.3497	679.5790
	C	0.677973	0.813792	-0.047541	691.4373	723.1052	735.5224
	C	-0.748180	3.241297	0.194787	755.4312	768.5988	782.6559
	C	1.297405	2.062642	-0.320447	787.9499	797.6326	806.9141
	C	0.552377	3.269354	-0.208376	821.6653	839.9804	857.4565
	C	2.681406	2.117828	-0.669802	866.6391	884.7875	900.0322
	C	3.457590	1.001039	-0.663334	937.6128	948.6799	961.6052
	C	1.562465	-0.316995	0.204167	968.4290	973.4934	980.5162
	C	2.935881	-0.227495	-0.168762	983.5940	999.0976	1000.6040
	C	3.796007	-1.347799	0.029675	1047.6943	1059.6087	1082.9569
	C	1.165610	-1.457500	0.947520	1092.2300	1147.0989	1164.6513
	C	2.042583	-2.488871	1.224210	1170.8536	1178.6858	1183.9149
	C	3.360718	-2.450431	0.755091	1185.0014	1207.4299	1222.7462
	H	-0.139561	-1.548348	-1.289014	1233.3699	1239.1393	1249.4128
	H	-4.828191	-1.459364	0.282310	1283.4825	1296.0348	1343.6977
	H	-4.596587	0.858635	0.960574	1352.2698	1362.1483	1375.3223
	H	-1.590295	-3.461249	-1.690712	1396.6649	1410.4680	1444.0620
	H	-3.932315	-3.476872	-0.834983	1448.2690	1460.5165	1470.0746
	H	-3.283691	2.946828	0.940347	1513.8613	1525.8701	1545.7011
	H	-1.295309	4.161032	0.371267	1552.0033	1585.7467	1619.1331
	H	1.057666	4.211217	-0.392484	1623.1026	1648.1871	1649.5638
H	3.100593	3.079409	-0.946217	1660.0740	3157.1910	3158.9652	

	H	4.499138	1.046106	-0.962390	3159.7601	3161.9095	3166.3569
	H	3.759216	-2.140019	-1.780784	3170.7669	3174.0605	3176.7994
	H	4.849621	-1.230268	-0.195690	3178.3302	3180.3640	3185.8035
	H	0.160109	-1.508908	1.338773	3189.7360	3216.7357	3218.4385
	H	1.706393	-3.328105	1.822376			
	H	4.040757	-3.269154	0.958744			
TS [i7]-p1	C	2.061256	-0.508632	-0.103972	-602.5422	56.1996	61.9073
	C	3.445930	-0.325133	0.214754	90.1569	121.2164	150.8247
	C	1.682954	-1.788777	-0.589923	192.8755	215.9640	251.6360
	C	1.159823	0.625189	-0.011139	256.4419	288.9515	310.3155
	C	4.330286	-1.429984	0.184206	322.0044	345.7137	400.0493
	C	3.939860	0.981560	0.491068	407.4204	419.6062	440.7707
	C	2.573896	-2.838641	-0.644934	475.8547	499.6234	507.9516
	C	1.730075	1.911124	0.110747	523.2941	533.6156	538.6144
	C	3.904614	-2.673350	-0.218672	570.4186	590.1839	601.2904
	C	3.121872	2.062857	0.379044	635.5027	650.7582	663.2392
	C	-0.298719	0.529930	-0.033279	713.5809	717.6549	746.4658
	C	0.919797	3.085789	-0.046928	757.4377	763.8715	780.5972
	C	-1.073932	1.730376	-0.249604	791.2173	806.3220	810.6429
	C	-0.409965	2.999807	-0.286026	817.8217	842.1356	847.9081
	C	-2.463385	1.660271	-0.337105	871.8558	883.4549	903.2796
	C	-3.160451	0.460660	-0.149971	917.0404	927.8432	949.1374
	C	-1.009826	-0.642502	0.244895	966.0316	972.8806	978.9767
	C	-2.407664	-0.709944	0.194235	983.2689	996.2913	1003.7999
	C	-3.120132	-1.921420	0.487494	1023.9583	1036.4318	1066.6979
	C	-4.579085	0.366274	-0.253177	1108.0412	1152.7218	1162.9216
	C	-5.222962	-0.826614	-0.037829	1170.9885	1181.4662	1183.3727
	C	-4.491341	-1.982904	0.318519	1194.0830	1212.9451	1229.6047
	H	0.687905	-1.937063	-0.980849	1235.7012	1253.8984	1284.4705
	H	5.367175	-1.267178	0.459254	1292.9961	1313.2272	1354.6305
	H	4.989454	1.102167	0.736802	1355.7754	1373.2701	1383.6349
	H	2.248477	-3.794835	-1.039170	1399.9776	1405.6948	1443.7121
	H	4.594582	-3.508884	-0.246759	1447.8166	1454.1950	1477.2169
	H	3.512397	3.065804	0.514415	1507.9401	1522.7811	1541.9841
	H	1.410591	4.052119	-0.001224	1565.4976	1583.8645	1616.7182
	H	-1.005184	3.891484	-0.450464	1631.2074	1648.3322	1653.6229
	H	-3.022034	2.572994	-0.520308	1668.6357	1655.7840	1657.5589
	H	-0.481699	-1.529481	0.562829	3159.3366	3160.8610	3161.5331
H	-2.551746	-2.827776	0.661028	3169.3415	3169.5889	3176.8540	
H	-3.091638	-1.863860	2.500104	3178.7707	3179.2259	3186.1456	
H	-5.142229	1.255116	-0.517414	3190.6942	3206.8512	3227.3671	
H	-6.300472	-0.888444	-0.139563				
H	-5.012992	-2.917778	0.486910				
[i3]	C	-1.982297	0.732554	-0.075879	21.2395	24.1016	58.2289
	C	-3.384833	0.869815	0.174265	78.2018	103.1504	122.7830
	C	-1.287085	1.906684	-0.466122	158.5216	178.2157	203.4617
	C	-1.379094	-0.590446	-0.019146	236.9210	269.2056	289.2218
	C	-3.979145	2.153349	0.178895	333.3684	355.0592	388.9071
	C	-4.191881	-0.294757	0.341400	394.9109	419.7895	431.7278
	C	-1.898595	3.142683	-0.488786	445.7084	450.8421	484.2696
	C	-2.248377	-1.708271	-0.010383	492.3126	529.8009	535.0711
	C	-3.250032	3.279060	-0.126708	544.4023	555.7667	589.6542
	C	-3.652114	-1.531690	0.188539	613.2199	633.1937	643.3473
	C	0.051198	-0.848958	0.031263	647.8110	687.8662	700.4169
	C	-1.734451	-3.027288	-0.197489	709.1923	745.6476	757.8593
	C	0.525660	-2.176480	-0.205709	768.7824	798.9641	809.5781
	C	-0.402795	-3.247507	-0.355037	812.5438	830.1681	840.5845
	C	1.917808	-2.430134	-0.213456	860.9246	877.1623	884.2315
	C	2.826643	-1.442355	0.074994	904.8475	928.0731	964.7478
	C	1.020823	0.118979	0.405520	969.7436	978.4163	982.4000
	C	2.375019	-0.153315	0.434544	988.5607	1001.8693	1022.3462
	C	3.378644	0.905931	0.859951	1037.0449	1067.0950	1128.4118
	C	4.276368	1.335683	-0.270991	1143.0428	1159.4657	1170.8152
	C	5.645898	1.288740	-0.215930	1179.2972	1183.7045	1185.7527
	C	6.865511	1.242296	-0.156578	1200.3158	1219.9078	1235.2628
	H	-0.266495	1.832028	-0.809058	1238.7740	1257.3189	1280.2597
	H	-5.038597	2.229681	0.400518	1294.9944	1326.6578	1351.8436
	H	-5.252136	-0.170812	0.534230	1369.9591	1383.7783	1397.4396
	H	-1.334421	4.011818	-0.808153	1400.2551	1430.9040	1449.8843
	H	-3.720517	4.255610	-0.128798	1461.7501	1472.5383	1477.7575

	H	-4.277303	-2.416790	0.239048	1526.5206	1538.8976	1555.5663
	H	-2.438747	-3.851532	-0.233690	1592.5336	1636.2499	1647.8613
	H	-0.022025	-4.246645	-0.537779	1652.4443	1666.2812	2014.2739
	H	2.257160	-3.438795	-0.425428	3001.7119	3065.2893	3150.6991
	H	3.890009	-1.655989	0.068594	3157.1752	3158.5165	3160.0505
	H	0.692814	1.091764	0.741487	3161.3548	3169.7875	3176.6117
	H	2.831095	1.777568	1.240987	3178.0857	3179.7016	3186.8458
	H	3.991288	0.533553	1.685712	3205.4623	3228.4039	3468.2338
	H	3.804655	1.694853	-1.180917			
	H	7.925971	1.206238	-0.109699			
[i4]	C	1.472103	0.861239	0.207059	19.4780	39.4353	69.6608
	C	2.719012	1.432532	-0.203689	80.3278	103.2524	122.9031
	C	0.568734	1.722519	0.883220	157.1682	179.2857	210.5676
	C	1.245584	-0.561077	0.005766	226.4332	267.5553	288.2578
	C	2.938768	2.823106	-0.066073	320.9013	354.9035	361.6898
	C	3.763235	0.585975	-0.680093	389.8245	422.9993	451.0569
	C	0.822678	3.069124	1.036241	465.1563	480.4362	510.4140
	C	2.364364	-1.365451	-0.316966	526.5091	535.3447	542.6870
	C	2.002297	3.638473	0.525462	550.1122	586.2226	587.7526
	C	3.609632	-0.763688	-0.673704	617.3693	638.9182	688.0493
	C	-0.049969	-1.219218	0.114109	690.1791	708.9712	740.1578
	C	2.266355	-2.790757	-0.287516	750.0528	757.3663	765.1666
	C	-0.096570	-2.649229	0.189775	787.4072	808.4512	813.5781
	C	1.096551	-3.409832	0.019275	822.4192	836.6289	845.2333
	C	-1.341215	-3.297759	0.352458	864.1973	884.3718	899.1424
	C	-2.518757	-2.590904	0.367118	935.3694	937.8177	940.5028
	C	-1.287206	-0.539154	0.050182	962.5188	967.7755	975.5575
	C	-2.506956	-1.190917	0.176699	982.0822	990.3153	1004.7153
	C	-3.795185	-0.470491	0.097759	1036.2228	1068.0129	1086.2453
	C	-3.973926	0.817592	-0.040450	1127.5073	1160.6706	1172.3220
	C	-4.195422	2.141332	-0.171268	1179.8724	1184.3798	1191.3625
	C	-4.328636	2.830531	-1.375266	1196.6447	1213.0002	1232.4877
	H	-0.319197	1.312847	1.339599	1238.0580	1255.4454	1276.9145
	H	3.882148	3.232228	-0.412542	1301.6351	1333.1144	1351.6447
	H	4.699087	1.037414	-0.991690	1368.1878	1384.5415	1397.1027
	H	0.111745	3.688231	1.571765	1405.9426	1435.9405	1450.5433
	H	2.187373	4.701122	0.633166	1459.7056	1476.5381	1490.6030
	H	4.428383	-1.413833	-0.963142	1526.5107	1538.4134	1556.4723
	H	3.160392	-3.369867	-0.492534	1589.9130	1633.4741	1647.6087
	H	1.039242	-4.491252	0.082016	1648.0005	1665.5020	1885.7004
	H	-1.353725	-4.379436	0.436595	3056.6608	3094.0999	3150.3189
	H	-3.465802	-3.106961	0.484279	3156.0548	3156.9382	3158.6799
	H	-1.304803	0.520027	-0.158462	3160.1043	3169.6600	3174.1132
H	-4.682356	-1.105499	0.164547	3176.2630	3178.5856	3185.7921	
H	-4.274412	2.716001	0.752414	3211.3228	3230.6473	3251.3962	
H	-4.258569	2.317031	-2.325451				
H	-4.502331	3.898292	-1.381149				
[i8]	C	-1.755607	0.896096	-0.063462	20.9817	27.1309	56.9319
	C	-3.117164	1.312026	0.076744	66.0382	86.2301	137.4484
	C	-0.789561	1.912667	-0.257482	141.7460	154.5241	179.9526
	C	-1.436470	-0.519890	-0.002513	236.7652	259.8497	271.9970
	C	-3.443625	2.687015	0.019143	326.8970	340.2527	361.9092
	C	-4.140979	0.338968	0.273610	399.9303	415.9753	417.8330
	C	-1.132168	3.246555	-0.309820	458.0292	467.5431	493.7751
	C	-2.491409	-1.441545	0.193323	511.6699	530.2973	539.4239
	C	-2.473830	3.643923	-0.170396	553.2599	592.8058	614.0117
	C	-3.837460	-0.983522	0.329162	635.1624	666.1809	677.2546
	C	-0.092801	-1.052622	-0.132193	681.5355	695.4415	711.7454
	C	-2.232840	-2.845518	0.258084	739.9492	746.0956	761.4166
	C	0.132691	-2.471417	-0.065137	768.8525	792.4811	808.4876
	C	-0.975510	-3.344825	0.133369	813.2809	834.9309	836.2980
	C	1.447284	-2.977962	-0.200521	857.4593	880.8906	901.7412
	C	2.529582	-2.150804	-0.394314	953.9014	958.5661	966.6080
	C	1.070157	-0.308488	-0.325982	971.3250	973.6158	982.3236
	C	2.355110	-0.742498	-0.464678	993.8194	1006.2757	1008.1213
	C	3.532057	0.190509	-0.640016	1051.8335	1067.4455	1118.8705
	C	5.318777	1.472149	0.563345	1154.2607	1170.0002	1176.1210
	C	6.264967	2.196377	0.407228	1180.8176	1184.2559	1209.6352
	C	4.165557	0.590644	0.717416	1220.5079	1240.2416	1242.8224
H	0.251463	1.630070	-0.369436	1261.7048	1288.7695	1294.5942	

	H	-4.484057	2.974884	0.128493	1311.5194	1341.7475	1362.6664
	H	-5.166549	0.676962	0.377583	1364.5727	1373.1040	1400.3637
	H	-0.360060	3.992724	-0.460246	1403.7846	1448.6434	1456.3538
	H	-2.738726	4.694297	-0.212591	1466.6627	1476.7498	1498.7916
	H	-4.617573	-1.722304	0.478366	1503.4406	1533.0828	1542.6234
	H	-3.074772	-3.512430	0.409965	1580.0393	1632.2273	1649.4265
	H	-0.794648	-4.413394	0.182862	1650.4145	1668.3215	2221.2532
	H	1.589841	-4.052245	-0.153417	3025.1199	3048.6983	3055.0933
	H	3.526181	-2.568541	-0.503767	3096.4008	3121.8277	3149.5636
	H	4.295649	-0.289124	-1.258328	3157.4501	3159.3990	3161.1150
	H	3.217725	1.096040	-1.162894	3171.7758	3173.7446	3176.9449
	H	7.102294	2.837369	0.279562	3179.4370	3186.9423	3477.9764
	H	4.466103	-0.312975	1.258803			
	H	3.406573	1.081635	1.335577			
	C	-1.818162	0.867495	-0.078652	19.8198	42.1695	55.2886
	C	-3.173138	1.230170	0.205970	81.4904	89.7401	122.2006
	C	-0.958251	1.909002	-0.514863	148.5408	177.3713	188.9169
	C	-1.430792	-0.533301	-0.008352	231.1882	273.1849	288.1513
	C	-3.556269	2.591736	0.198373	326.5804	343.4061	366.0330
	C	-4.149566	0.212089	0.419298	395.6506	409.1491	428.0798
	C	-1.367051	3.225687	-0.549289	444.5670	472.1702	486.2228
	C	-2.466085	-1.497688	0.044463	526.7462	531.0622	548.5695
	C	-2.667910	3.581539	-0.152802	549.6976	591.6528	627.0072
	C	-3.817717	-1.097049	0.276880	636.1418	665.3452	675.2979
	C	-0.057317	-1.014395	0.009547	676.2206	695.4954	706.6086
	C	-2.174400	-2.883620	-0.133697	744.9136	755.2180	760.3557
	C	0.188793	-2.406072	-0.218573	770.3278	793.2248	808.9366
	C	-0.900657	-3.317696	-0.324685	811.9793	831.4667	844.0347
	C	1.530253	-2.883481	-0.256811	870.5817	883.0316	894.4295
	C	2.523982	-2.001320	0.001244	919.1696	964.7567	967.1339
	C	1.056260	-0.197068	0.344117	969.5426	977.5950	982.3796
	C	2.365250	-0.662576	0.352579	1002.0017	1009.0660	1018.3519
	C	3.531655	0.218425	0.732772	1040.8558	1069.0899	1125.7692
	C	5.610259	1.337193	-0.107213	1164.6023	1169.1462	1181.4715
	C	6.534653	2.035732	0.211667	1182.6597	1194.2369	1212.4835
	C	4.474766	0.492985	-0.465069	1229.1079	1234.7032	1245.2618
	H	0.026341	1.667377	-0.885265	1266.4937	1283.5869	1302.5603
	H	-4.582920	2.839083	0.447532	1315.4997	1338.4331	1360.7314
	H	-5.170413	0.506303	0.638000	1369.5843	1377.1486	1396.1896
	H	-0.682819	3.988139	-0.904337	1400.2489	1437.8806	1452.5145
	H	-2.977598	4.620242	-0.164072	1463.9301	1476.8525	1494.9042
	H	-4.573547	-1.870567	0.361337	1501.4113	1529.9166	1545.5781
	H	-3.001592	-3.585430	-0.136423	1581.6110	1617.8564	1640.2484
	H	-0.689702	-4.366820	-0.500826	1647.7478	1663.5207	2221.5530
	H	1.716785	-3.933935	-0.455878	3023.4189	3044.0567	3052.4921
	H	0.887610	0.818987	0.672491	3090.6871	3158.0477	3158.8592
	H	3.164320	1.168918	1.126695	3160.4280	3162.3529	3170.6773
	H	4.112105	-0.256463	1.529041	3178.0670	3180.4242	3186.9068
	H	7.355901	2.651415	0.485051	3198.8952	3226.1590	3476.9764
	H	3.906609	0.967230	-1.272749			
	H	4.837583	-0.461196	-0.862022			
	C	-1.588146	-0.393687	0.167637	63.1872	73.2836	86.4047
	C	-2.971867	-0.369241	-0.194111	117.5067	147.6835	168.4763
	C	-1.116026	-1.547214	0.843706	200.9870	238.6904	267.5989
	C	-0.773602	0.789363	-0.047010	287.7063	321.2578	343.7794
	C	-3.765473	-1.526450	-0.011967	389.1260	397.0494	415.5350
	C	-3.557968	0.848333	-0.649330	442.4055	459.5324	483.3620
	C	-1.922003	-2.645706	1.048042	496.4862	502.5151	532.3535
	C	-1.454691	2.008884	-0.279629	545.4033	552.5624	564.2764
	C	-3.251057	-2.653846	0.585422	608.7874	614.5937	656.2210
	C	-2.840259	2.003221	-0.625373	685.0198	691.6739	711.0571
	C	0.679378	0.828379	0.050919	740.4134	756.2370	767.8154
	C	-0.774862	3.254114	-0.113731	783.6077	785.4028	802.7958
	C	1.288071	2.084910	0.369028	812.7760	834.9119	855.8864
	C	0.519417	3.286429	0.296803	860.5552	863.0311	882.6500
	C	2.665190	2.143210	0.665803	902.3280	937.9058	948.3268
	C	3.455206	1.022190	0.560262	956.8788	963.8812	970.6100
	C	1.556966	-0.268066	-0.240471	979.3549	985.4667	995.4072
	C	2.924294	-0.175330	0.054006	1016.8923	1047.8895	1069.5929
	C	3.869030	-1.305707	-0.313474	1073.4889	1150.0530	1168.5542

	C	1.893304	-2.540198	-0.995287	1170.8699	1173.9436	1182.6057
	C	1.117445	-1.472427	-0.994199	1188.7820	1196.3334	1217.9568
	C	3.196723	-2.696417	-0.313347	1229.4629	1237.6615	1242.4905
	H	-0.108868	-1.554490	1.233470	1248.4936	1277.5929	1306.6401
	H	-4.804724	-1.494466	-0.322364	1325.5912	1341.2439	1359.0647
	H	-4.603099	0.849616	-0.939992	1362.0801	1382.9805	1389.5904
	H	-1.529770	-3.505772	1.578815	1406.0505	1443.1317	1450.3539
	H	-3.873359	-3.529266	0.732568	1463.6902	1467.9598	1473.8603
	H	-3.309616	2.949662	-0.872307	1522.8943	1526.9296	1554.1670
	H	-1.334753	4.171703	-0.259113	1581.6853	1617.3194	1637.3995
	H	1.012120	4.228547	0.511926	1647.3053	1661.5135	1684.0870
	H	3.097409	3.095946	0.952350	2988.8502	2999.0710	3057.1185
	H	4.513599	1.077891	0.793485	3059.3449	3155.8585	3157.1652
	H	4.256559	-1.111216	-1.322743	3159.3455	3160.9640	3171.1843
	H	4.731579	-1.305278	0.359610	3174.8587	3176.8820	3178.5392
	H	0.177599	-1.437042	-1.531272	3180.0021	3186.4377	3220.4690
	H	3.038243	-3.057635	0.712479			
	H	3.842648	-3.426671	-0.809114			
	C	-1.620978	-0.406917	-0.187939			
	C	-2.996907	-0.384326	0.202833	60.5803	72.4599	94.3599
	C	-1.174805	-1.538554	-0.918114	110.7395	148.4704	170.2267
	C	-0.789977	0.758339	0.059368	200.8996	233.8469	269.4707
	C	-3.807344	-1.524035	-0.014208	281.8038	316.8027	350.6178
	C	-3.559519	0.815906	0.727752	369.9577	403.3801	414.3677
	C	-1.996935	-2.618433	-1.153486	441.2227	465.0887	482.6106
	C	-1.452204	1.971055	0.365496	486.4337	517.3034	529.0945
	C	-3.318465	-2.630344	-0.669052	544.6693	551.8793	563.3616
	C	-2.828899	1.962797	0.744140	609.3955	624.9437	655.4996
	C	0.659518	0.791208	-0.092183	686.0112	702.8498	711.5533
	C	-0.765169	3.217660	0.237266	741.2013	755.9226	767.6273
	C	1.266654	2.056123	-0.383631	785.1053	792.5665	794.9954
	C	0.512726	3.259033	-0.219407	813.4800	835.1999	853.0667
	C	2.626943	2.118242	-0.744445	856.8479	860.6949	884.2095
	C	3.403988	0.980971	-0.751593	900.1224	935.6087	951.9478
	C	1.539069	-0.321810	0.108247	954.2983	964.0801	970.9982
	C	2.884287	-0.233631	-0.283242	979.0136	980.9565	997.4679
	C	3.767185	-1.464726	-0.208256	1023.8976	1047.0090	1067.9697
	C	2.086777	-2.352619	1.315551	1073.8323	1150.3563	1169.4297
	C	1.149943	-1.517911	0.904598	1170.9311	1173.8860	1183.0827
	C	3.542981	-2.295224	1.080563	1190.2024	1197.3469	1217.2925
	H	-0.172078	-1.544355	-1.321215	1229.4312	1240.5303	1245.1238
	H	-4.839824	-1.494257	0.318199	1250.0809	1281.3115	1309.0612
	H	-4.598073	0.813942	1.040957	1321.5650	1338.7913	1360.6319
	H	-1.623674	-3.460349	-1.725491	1362.5997	1381.9924	1390.7972
	H	-3.954054	-3.491354	-0.841894	1407.4156	1442.1422	1450.3927
	H	-3.281868	2.900999	1.046813	1467.4693	1470.1817	1480.3893
	H	-1.310886	4.131731	0.445162	1521.7482	1528.6072	1555.2117
	H	1.005987	4.206431	-0.408554	1583.0583	1616.5319	1636.5493
	H	3.057901	3.081432	-0.995412	1647.6369	1662.1176	1686.7008
	H	4.444671	1.033167	-1.054316	2992.6225	3002.4995	3057.0897
	H	3.533402	-2.109208	-1.065739	3066.9040	3156.0036	3156.6620
	H	4.820440	-1.185639	-0.296660	3158.5888	3159.9949	3169.9325
	H	0.123781	-1.626758	1.227683	3174.5224	3176.2784	3178.8807
	H	4.031880	-1.825638	1.945271	3185.2751	3196.3133	3210.7266
	H	3.989186	-3.286966	0.963648			
	C	2.057396	-0.501917	-0.100237	54.0698	60.5808	91.6892
	C	3.427514	-0.322209	0.272398	113.9806	140.3823	176.4143
	C	1.701754	-1.771189	-0.625884	200.6312	235.2587	271.8463
	C	1.147176	0.631583	-0.021996	284.9441	314.7446	330.5106
	C	4.313886	-1.424400	0.256879	383.5519	400.3906	411.6034
	C	3.912360	0.983597	0.581693	427.8837	445.9066	478.9992
	C	2.595611	-2.820962	-0.665037	491.5455	514.6869	536.1300
	C	1.717137	1.919819	0.129533	541.9846	563.7318	578.1798
	C	3.906793	-2.662288	-0.184025	598.3350	637.1129	644.7234
	C	3.101881	2.065429	0.448337	692.3128	712.8424	715.1647
	C	-0.300766	0.539610	-0.089508	745.5476	759.0816	764.3579
	C	0.914171	3.089249	-0.030022	767.1900	805.8526	810.9232
	C	-1.065742	1.730043	-0.292590	814.1109	829.1399	838.9731
	C	-0.415606	2.999079	-0.295686	850.2073	883.2867	891.5172
	C	-2.471806	1.651414	-0.405682	906.3937	923.2191	931.6986

	C	-3.150200	0.459409	-0.255768	944.6735	964.7687	974.2282
	C	-1.035520	-0.657703	0.129161	978.2221	981.8393	1001.3788
	C	-2.408929	-0.719255	0.046251	1018.8911	1024.3488	1067.6632
	C	-3.151430	-2.032905	0.196908	1102.5328	1155.8036	1171.4566
	C	-5.207645	-0.692691	0.211096	1174.4265	1178.8858	1183.0841
	C	-4.625612	0.378294	-0.298145	1202.3748	1206.5237	1221.5723
	C	-4.560225	-1.872907	0.826140	1231.0523	1242.7774	1250.6538
	H	0.724348	-1.912319	-1.061252	1257.7443	1282.8717	1319.0821
	H	5.339541	-1.264937	0.573082	1322.8779	1345.3584	1355.1463
	H	4.952603	1.099577	0.866437	1371.4460	1382.5714	1396.7030
	H	2.286995	-3.769672	-1.089834	1418.1554	1450.4548	1463.9677
	H	4.599609	-3.495861	-0.200175	1467.0972	1476.5270	1482.7179
	H	3.487762	3.066813	0.607272	1513.8845	1534.5134	1545.6278
	H	1.397735	4.057450	0.044895	1590.8113	1633.9753	1647.3121
	H	-1.012281	3.890921	-0.454513	1648.4962	1664.5696	1684.7653
	H	-3.028232	2.568793	-0.572452	2998.5249	3006.8921	3057.2518
	H	-0.508206	-1.555172	0.417820	3067.5429	3145.0094	3155.5888
	H	-3.280727	-2.466960	-0.803079	3157.6368	3159.5611	3161.0323
	H	-2.559691	-2.745068	0.778472	3169.6367	3176.9523	3179.1455
	H	-5.183384	1.223010	-0.692480	3186.4083	3204.7391	3227.7838
	H	-4.489976	-1.723190	1.911776			
	H	-5.139288	-2.787989	0.671140			
	C	1.592703	-0.391021	-0.194272	61.5776	68.7656	89.1101
	C	2.973605	-0.372133	0.174027	97.8596	124.1437	170.6259
	C	1.129370	-1.527036	-0.906175	201.5465	242.7113	258.5418
	C	0.770087	0.784351	0.052971	290.1842	313.6863	346.3700
	C	3.774084	-1.519804	-0.039510	393.1114	417.2735	438.9533
	C	3.554977	0.832681	0.669942	454.4587	466.7266	488.0715
	C	1.941364	-2.615278	-1.140237	498.7294	523.6153	534.3683
	C	1.449381	1.998053	0.328628	540.9088	555.7426	598.9485
	C	3.268873	-2.631235	-0.672903	610.1381	626.1136	663.7311
	C	2.833900	1.984909	0.679716	675.0988	688.1840	697.6567
	C	-0.677835	0.825596	-0.056367	716.2255	754.3514	759.8619
	C	0.766958	3.245278	0.211014	780.7061	782.7588	789.6457
	C	-1.287113	2.086885	-0.328137	804.6892	817.7652	838.9143
	C	-0.527562	3.288257	-0.200131	854.3714	861.9650	881.7588
	C	-2.659893	2.151324	-0.661019	922.3340	930.5074	943.5773
	C	-3.438004	1.016421	-0.656217	957.3939	961.8735	963.8389
	C	-1.561138	-0.300649	0.179776	967.7696	969.7161	978.4541
	C	-2.919702	-0.204131	-0.201925	994.8831	1046.0932	1063.2654
	C	-3.852647	-1.392495	-0.083034	1071.7516	1115.6506	1153.3498
	C	-1.154184	-1.447819	0.934192	1169.0650	1175.3808	1179.9272
	C	-2.038401	-2.511284	1.203710	1182.8703	1194.4861	1201.3628
	C	-3.316581	-2.528401	0.728465	1206.3967	1231.8169	1241.0076
	H	0.122707	-1.530711	-1.297598	1245.3722	1261.6730	1291.5445
	H	4.811721	-1.491705	0.276615	1294.9750	1343.3477	1356.1091
	H	4.599016	0.827439	0.964300	1371.6883	1385.5589	1397.4768
	H	1.555353	-3.460053	-1.699568	1410.8031	1427.6795	1446.9375
	H	3.896522	-3.498447	-0.844126	1448.6890	1461.8540	1470.5073
	H	3.298886	2.924434	0.959247	1519.8608	1528.0215	1549.4078
	H	1.322728	4.158504	0.394740	1563.9244	1582.5301	1608.2515
	H	-1.023957	4.235842	-0.379728	1633.9187	1647.5407	1660.6848
	H	-3.092198	3.115138	-0.906903	2913.7769	2981.0136	3152.0201
	H	-4.485402	1.075868	-0.935505	3154.5640	3156.1663	3158.1428
	H	-4.817152	-1.061373	0.327493	3159.7757	3169.2566	3173.5146
	H	-4.102730	-1.752537	-1.097238	3175.3757	3176.0739	3178.7778
	H	-0.163628	-1.474303	1.361479	3184.7501	3217.5844	3226.9199
	H	-1.681340	-3.335881	1.812319			
	H	-3.973982	-3.367031	0.929400			
	C	2.061343	-0.515061	-0.096935	42.1541	61.5713	80.4764
	C	3.445160	-0.341092	0.224868	103.6904	124.0656	164.3535
	C	1.675393	-1.791376	-0.582193	209.8928	228.8828	262.7026
	C	1.164844	0.628919	-0.012648	287.2977	318.8006	338.8615
	C	4.320323	-1.452150	0.201323	391.1733	407.7093	422.6976
	C	3.951592	0.965694	0.490886	446.1893	473.3271	487.0452
	C	2.557795	-2.850561	-0.630481	500.1022	519.9774	537.3973
	C	1.751444	1.915007	0.093930	550.9198	573.5804	593.2694
	C	3.886712	-2.694579	-0.199740	607.3671	635.9233	647.6405
	C	3.146049	2.053042	0.363518	663.9331	691.7298	713.6707
	C	-0.283229	0.548969	-0.029952	715.8284	754.4605	762.3306

	C	0.952913	3.089583	-0.063092	763.4713	781.6761	805.3775
	C	-1.047616	1.743635	-0.236108	808.7060	816.5094	839.3434
	C	-0.384349	3.007665	-0.284730	846.4024	881.8499	891.4394
	C	-2.447638	1.670189	-0.320450	904.7800	908.4891	942.3073
	C	-3.146780	0.477671	-0.133522	953.0943	954.8063	963.7839
	C	-1.020788	-0.634192	0.243445	966.8846	975.1235	980.7365
	C	-2.395464	-0.693601	0.201815	1002.8114	1022.2059	1067.0082
	C	-3.114556	-1.988480	0.535341	1072.6021	1125.2633	1162.2230
	C	-4.572746	0.408883	-0.226397	1171.2860	1172.8186	1182.4290
	C	-5.258664	-0.795277	0.009077	1188.5690	1198.4116	1205.7679
	C	-4.602338	-1.942190	0.364377	1223.5357	1230.6811	1243.7941
	H	0.681362	-1.931611	-0.978822	1257.0610	1289.8000	1305.4466
	H	5.357772	-1.296550	0.478622	1320.6272	1344.3833	1354.0761
	H	5.001896	1.077748	0.737708	1372.5395	1386.6154	1398.0658
	H	2.225716	-3.805018	-1.023526	1423.6947	1443.7987	1446.6507
	H	4.570974	-3.535032	-0.223009	1450.4148	1465.1837	1473.4725
	H	3.546587	3.053408	0.489415	1517.4835	1534.1840	1543.3468
	H	1.447943	4.054120	-0.023967	1561.9910	1586.7920	1625.9708
	H	-0.977617	3.901632	-0.444331	1631.5478	1646.9381	1663.2621
	H	-3.003845	2.583649	-0.508179	2952.6310	2976.7814	3154.0658
	H	-0.488611	-1.522997	0.552330	3155.3532	3157.2570	3159.2396
	H	-2.701044	-2.805967	-0.073278	3160.7993	3169.2224	3172.0154
	H	-2.879372	-2.277403	1.572435	3176.7726	3178.9677	3182.8012
	H	-5.122234	1.306488	-0.485754	3186.0736	3197.5094	3225.1270
	H	-6.339326	-0.810275	-0.090097			
	H	-5.156597	-2.856378	0.546474			
	C	-1.273969	-0.281465	0.050973			
	C	-2.448402	0.503591	-0.178006	79.0980	83.9753	128.1870
	C	-1.474592	-1.638515	0.414493	177.9813	211.4427	260.0142
	C	0.028722	0.364520	-0.000773	278.6239	325.1728	377.9785
	C	-3.720555	-0.114427	-0.186856	411.5753	438.3818	441.1265
	C	-2.337853	1.918854	-0.320386	477.4310	510.9803	525.5294
	C	-2.730084	-2.209316	0.432813	526.7403	552.4507	575.1484
	C	0.063747	1.779995	0.011437	593.2032	623.4733	672.6080
	C	-3.865463	-1.453409	0.093222	686.4891	703.7541	749.1795
	C	-1.136683	2.533814	-0.166146	757.1880	758.8876	776.4242
	C	1.298349	-0.338621	-0.067416	805.3191	824.4209	826.2772
	C	1.297945	2.472676	0.200413	851.4441	855.0845	877.5391
	C	2.514109	0.383060	0.168622	896.1644	952.4505	958.3356
	C	2.469545	1.799122	0.338041	966.7867	975.1529	982.8406
	C	3.763334	-0.284414	0.158659	1002.0446	1012.6423	1057.1376
	C	3.862465	-1.631340	-0.138003	1078.6439	1122.1064	1145.3288
	C	1.433077	-1.706085	-0.461674	1171.2432	1174.9236	1183.9830
	C	2.671335	-2.263196	-0.460788	1205.1101	1223.3171	1235.4796
	H	-0.635934	-2.234068	0.741140	1245.9869	1263.5857	1307.8496
	H	-4.590739	0.500608	-0.391349	1343.0963	1351.1362	1369.1997
	H	-3.238885	2.496481	-0.496887	1394.5929	1410.0419	1439.6083
	H	-2.840349	-3.245859	0.731017	1451.8378	1472.0577	1499.0507
	H	-4.847313	-1.912669	0.092076	1530.4077	1545.5977	1588.5720
	H	-1.061968	3.615493	-0.199122	1611.9531	1635.9618	1647.8789
	H	1.274918	3.555776	0.254148	1665.4207	3153.5571	3157.4577
	H	3.396815	2.331023	0.521542	3159.5646	3161.1358	3170.1760
	H	4.659181	0.291608	0.369653	3176.8116	3179.2223	3181.0244
	H	4.817602	-2.143189	-0.143273	3186.4303	3202.3191	3227.6458
	H	0.576509	-2.264272	-0.810689			
	C	2.047374	-1.219444	-0.300457	4.7337	10.2313	10.9347
	C	2.908689	-2.248367	0.189588	25.3461	32.8382	46.7352
	C	1.147947	-1.570127	-1.338191	67.0739	73.3060	91.5319
	C	2.222848	0.147402	0.175812	121.2898	172.7069	178.0729
	C	2.733262	-3.581469	-0.251722	228.1770	231.9721	246.1581
	C	4.000351	-1.909133	1.045447	278.7616	313.1916	319.2710
	C	1.025402	-2.868610	-1.782562	343.7574	399.5834	413.3331
	C	3.448462	0.447850	0.826612	419.6677	450.2333	470.1292
	C	1.799463	-3.895636	-1.211590	478.0634	496.9802	518.5379
	C	4.294331	-0.606589	1.292800	538.1107	545.7541	552.4314
	C	1.290713	1.235269	-0.043342	559.6726	567.3789	611.7140
	C	3.862148	1.799682	0.983135	626.3073	643.4824	650.4952
	C	1.800208	2.561197	-0.021161	673.5063	680.2990	691.4188
	C	3.105661	2.815833	0.482773	703.2950	717.3903	727.5107
	C	0.990973	3.652680	-0.465000	756.9544	767.2692	775.4715

	C	-0.306571	3.470252	-0.821631	782.3808	791.5710	810.1857
	C	-0.151665	1.089435	-0.186787	822.4485	839.0149	856.7963
	C	-0.934378	2.201359	-0.630816	860.1590	880.7933	884.8780
	C	-0.862026	-0.076543	0.229969	892.1123	931.6858	944.8645
	C	-2.209268	-0.100181	0.070419	956.2706	962.8736	966.1089
	C	-3.002113	0.911966	-0.451929	969.1217	976.3759	981.0508
	C	-2.337127	2.076552	-0.788872	999.1745	1009.2955	1048.0978
	H	0.554706	-0.799169	-1.807769	1063.1933	1082.6218	1091.9631
	H	3.379441	-4.350510	0.158568	1112.2884	1145.9897	1161.0689
	H	4.633128	-2.704007	1.425388	1173.3390	1178.7202	1184.3500
	H	0.333125	-3.095715	-2.585298	1201.2364	1215.1579	1228.9562
	H	1.684268	-4.918433	-1.551817	1233.4323	1244.5342	1268.4498
	H	5.181795	-0.337626	1.855777	1287.3929	1321.8502	1323.0475
	H	4.818477	1.998863	1.454517	1343.1439	1359.4951	1374.3827
	H	3.458770	3.840782	0.516260	1389.5037	1403.2926	1414.9798
	H	1.442825	4.637774	-0.510561	1442.7133	1446.3845	1450.6503
	H	-0.905716	4.300270	-1.180050	1467.3981	1497.0399	1513.7432
	H	-0.333083	-0.906775	0.677067	1536.2375	1549.3456	1582.7413
	H	-4.075433	0.812725	-0.565248	1610.0926	1621.4819	1648.3463
	H	-2.895471	2.932486	-1.155645	1653.4916	1660.5930	1668.2289
	C	-5.429048	-1.426779	2.100264	2201.8700	3134.8689	3143.4899
	C	-6.597344	-1.157841	1.508231	3153.5720	3157.2348	3158.9934
	C	-6.743076	-0.779198	0.144162	3159.8147	3161.7830	3171.0873
	C	-6.909738	-0.457236	-1.005087	3176.6923	3177.9280	3180.1113
	H	-5.391718	-1.708609	3.145592	3180.7581	3186.1448	3200.0095
	H	-4.489016	-1.369613	1.563774	3217.7612	3233.1486	3476.4033
	H	-7.519356	-1.223878	2.080748			
	H	-7.049601	-0.182515	-2.021679			
p7	C	1.588285	-0.544702	-0.499249			
	C	2.840640	-1.167607	-0.210020	47.6776	67.5148	68.7063
	C	0.734260	-1.203774	-1.416287	104.2938	113.8247	130.8369
	C	1.293987	0.765153	0.066848	180.0381	194.9433	246.0667
	C	3.129331	-2.446895	-0.740130	252.8712	258.8954	309.9693
	C	3.823678	-0.463051	0.550021	321.0205	369.0303	407.2560
	C	1.054950	-2.433294	-1.949598	421.7123	427.6531	436.2217
	C	2.382659	1.492757	0.613627	436.8204	474.8415	488.3495
	C	2.250236	-3.080010	-1.588111	512.3939	519.7071	530.2985
	C	3.620996	0.834590	0.894704	534.0044	546.0432	568.5214
	C	0.000000	1.422446	-0.000002	575.5197	619.9768	633.4147
	C	2.270898	2.894945	0.830728	645.4641	669.6508	688.7904
	C	0.000000	2.848382	-0.000004	705.2322	708.1572	751.2725
	C	1.151403	3.561787	0.436519	752.8798	756.8058	757.0350
	C	-1.151402	3.561786	-0.436528	768.2905	783.6581	805.3933
	C	-2.270897	2.894943	-0.830735	812.8710	817.8606	838.4626
	C	-1.293986	0.765153	-0.066850	841.6048	844.2637	859.4332
	C	-2.382659	1.492756	-0.613631	883.8664	884.6595	914.9288
	C	-1.588285	-0.544700	0.499251	929.7106	957.0747	963.3306
	C	-2.840640	-1.167605	0.210022	966.2949	969.3604	977.9604
	C	-3.823678	-0.463051	-0.550020	979.3353	996.8830	996.9297
	C	-3.620996	0.834589	-0.894707	998.4022	1052.6606	1062.1186
	C	-0.734260	-1.203770	1.416291	1068.1832	1113.7163	1137.7759
	C	-1.054951	-2.433288	1.949605	1164.4713	1165.8570	1177.8412
	C	-2.250237	-3.080005	1.588119	1178.5170	1184.6376	1185.4671
	C	-3.129331	-2.446893	0.740136	1205.7105	1211.0793	1231.4355
	H	-0.182533	-0.724281	-1.725847	1233.3410	1241.2520	1246.4316
	H	4.078050	-2.908846	-0.487143	1277.1503	1300.0189	1318.8713
	H	4.759427	-0.960254	0.782273	1357.1226	1359.0895	1369.9807
	H	0.380224	-2.900724	-2.657750	1382.0713	1384.7201	1393.1290
	H	2.488123	-4.055199	-1.997620	1421.0343	1448.9792	1449.7611
	H	4.401650	1.404433	1.387455	1465.9883	1471.3663	1506.6575
	H	3.123657	3.428621	1.236081	1516.6303	1537.5281	1548.0872
	H	1.102216	4.644317	0.483112	1557.2340	1586.3534	1613.5793
	H	-1.102215	4.644316	-0.483124	1641.6198	1648.7934	1648.8681
	H	-3.123656	3.428618	-1.236090	1660.3646	1661.1276	3156.1593
	H	-4.759427	-0.960255	-0.782271	3156.2803	3158.2366	3158.5004
	H	-4.401650	1.404430	-1.387459	3159.9732	3161.8142	3170.2632
	H	0.182532	-0.724276	1.725850	3170.3468	3175.8804	3176.3154
	H	-0.380225	-2.900716	2.657758	3178.5207	3180.3782	3185.2294
H	-2.488124	-4.055193	1.997631	3185.5148	3219.5594	3219.7894	
H	-4.078051	-2.908845	0.487149				

p8	C	-1.832937	-0.998898	0.296910			
	C	-2.893943	-1.845577	-0.145389	43.9662	58.5227	69.2432
	C	-0.906833	-1.552054	1.215519	95.5722	118.8082	144.7491
	C	-1.828187	0.408562	-0.093855	171.2249	198.6926	231.1436
	C	-2.897694	-3.214572	0.212631	264.4361	278.5598	294.2637
	C	-3.995708	-1.285749	-0.863297	330.0936	353.7998	395.3912
	C	-0.955756	-2.879182	1.584437	408.4953	412.7214	443.1424
	C	-3.049930	0.937753	-0.594787	452.4389	478.2228	484.0898
	C	-1.939324	-3.732914	1.052514	499.8588	521.1562	534.0291
	C	-4.097499	0.058860	-1.016274	537.1135	554.1671	566.5979
	C	-0.717352	1.318785	0.068790	592.0134	614.4769	636.9766
	C	-3.249431	2.341530	-0.651788	641.7277	650.4817	693.2826
	C	-1.001327	2.704430	0.152795	704.5229	715.8527	751.1980
	C	-2.286001	3.194194	-0.197056	754.2833	759.8867	769.8406
	C	0.015894	3.629767	0.572268	778.3969	782.9217	797.8233
	C	1.287638	3.229062	0.803524	812.3772	814.8198	832.0212
	C	0.698747	0.935180	0.055147	842.6365	854.1828	860.4706
	C	1.691403	1.887779	0.493107	884.3920	899.7749	907.2767
	C	1.157689	-0.264405	-0.486991	926.1849	935.0868	951.6070
	C	2.516704	-0.615294	-0.506998	961.6142	968.4322	970.1431
	C	3.486247	0.291532	0.040809	977.5409	981.0529	995.0005
	C	3.038794	1.532706	0.511955	999.0252	1032.2676	1052.4463
	C	4.860585	-0.086115	0.038025	1073.6034	1097.3724	1144.3001
	C	4.297312	-2.183467	-1.035219	1163.3477	1167.1197	1176.5169
	C	5.254731	-1.289302	-0.482792	1182.0295	1183.9777	1193.8578
	C	2.968451	-1.854379	-1.049230	1210.3106	1213.6387	1230.1000
	H	-0.151321	-0.916218	1.653104	1242.6741	1252.9046	1286.8331
	H	-3.698515	-3.843873	-0.161577	1290.5821	1304.0846	1323.8607
	H	-4.783232	-1.946423	-1.209595	1355.5274	1360.1935	1365.6852
	H	-0.235269	-3.262218	2.298214	1374.3294	1401.6167	1417.9003
	H	-1.961371	-4.780307	1.331267	1420.5785	1444.9570	1448.6197
	H	-4.980139	0.498587	-1.468484	1461.3299	1473.3087	1507.0046
	H	-4.201059	2.718378	-1.010602	1509.5331	1536.5146	1543.9566
	H	-2.466442	4.262744	-0.151659	1575.2281	1591.1197	1616.2376
	H	-0.270599	4.666584	0.713254	1630.8063	1648.4986	1655.9334
	H	2.038545	3.930507	1.150790	1662.1246	1667.2697	3154.3064
H	0.452106	-0.962611	-0.915439	3156.8163	3157.4054	3158.4012	
H	3.766454	2.259444	0.860204	3159.2342	3161.4645	3163.2820	
H	5.590862	0.600513	0.453520	3170.5998	3175.1565	3176.4001	
H	4.627851	-3.131004	-1.445517	3177.4882	3179.8280	3185.6742	
H	6.302941	-1.566487	-0.479911	3187.0506	3204.3135	3218.8564	
H	2.235552	-2.537007	-1.466102				
p6	C	0.653351	1.589881	0.455673	26.6117	49.6650	62.3632
	C	0.694225	2.964124	0.069542	77.7355	85.8940	97.7489
	C	-0.250871	1.236058	1.488500	120.2468	149.9432	159.0209
	C	1.617421	0.656568	-0.116512	195.0519	231.1975	246.7148
	C	-0.252746	3.872305	0.600353	262.9823	308.3415	316.7935
	C	1.747576	3.431131	-0.774583	341.4399	360.1521	412.4969
	C	-1.135157	2.148909	2.021593	418.0610	421.6084	442.8873
	C	2.757201	1.220157	-0.749598	465.2386	471.5740	485.4858
	C	-1.164775	3.474753	1.550188	496.3746	515.4367	540.8646
	C	2.771705	2.604447	-1.108404	543.3486	557.0344	574.9316
	C	1.548299	-0.786249	-0.011929	602.2982	617.8308	622.3446
	C	3.906072	0.420040	-0.997632	641.0551	670.0274	678.1529
	C	2.760003	-1.518166	-0.121477	689.2019	692.7632	721.6734
	C	3.937893	-0.883294	-0.602515	736.1476	758.2297	772.6837
	C	2.797022	-2.907811	0.215352	777.3964	794.1536	798.4457
	C	1.668146	-3.584003	0.553102	812.4392	830.9195	843.7892
	C	0.317523	-1.564315	0.102748	855.1405	860.8658	877.9652
	C	0.395206	-2.949970	0.444348	885.1241	891.7040	926.3439
	C	-0.949905	-1.050568	-0.244272	947.3942	960.6241	966.2107
	C	-2.116687	-1.801237	-0.149780	970.1345	977.7464	981.7570
	C	-2.020021	-3.145249	0.292105	989.9029	996.5419	999.7722
	C	-0.796696	-3.701100	0.569190	1036.5552	1055.6947	1087.2517
	C	-3.436122	-1.274603	-0.499179	1095.6729	1154.1764	1169.2656
	C	-3.762043	0.015358	-0.719048	1176.2591	1181.9295	1184.3435
	C	-5.067308	0.446674	-1.061100	1203.9502	1206.1437	1222.0271
	C	-6.167065	0.848035	-1.351168	1231.6710	1242.0782	1251.2799
	H	-0.236225	0.230878	1.883824	1287.5406	1294.5513	1312.1252
	H	-0.221646	4.904331	0.266937	1331.8278	1348.2736	1358.6047

	H	1.753367	4.473359	-1.074951	1368.0432	1374.1333	1400.3699
	H	-1.804666	1.842955	2.817368	1413.8674	1429.8024	1449.3874
	H	-1.876524	4.182765	1.958947	1464.7904	1471.3231	1509.3317
	H	3.626157	2.978907	-1.662021	1527.2938	1545.4827	1551.8057
	H	4.774126	0.884230	-1.452992	1583.7047	1617.9173	1640.4829
	H	4.842077	-1.473497	-0.704424	1648.0794	1652.7319	1659.7660
	H	3.757657	-3.411372	0.197023	1670.5952	2193.6163	3142.6841
	H	1.709047	-4.631411	0.831827	3151.3591	3157.8606	3158.3442
	H	-1.009570	-0.042627	-0.626766	3159.8764	3160.6127	3162.2801
	H	-2.922501	-3.740422	0.381068	3172.0991	3176.1784	3177.4260
	H	-0.723685	-4.745034	0.855358	3178.5746	3180.6185	3187.1867
	H	-4.230516	-2.012818	-0.568364	3217.1871	3218.9843	3477.6788
	H	-3.012345	0.796362	-0.626995			
	H	-7.138219	1.192141	-1.608824			
	C	0.866579	1.560552	0.459315			
	C	1.017361	2.926930	0.071711	25.8869	36.9318	48.5026
	C	-0.032163	1.285900	1.520208	69.5628	81.0340	88.5517
	C	1.725898	0.547385	-0.142621	121.2352	152.6198	158.6976
	C	0.174621	3.914692	0.634514	193.3159	221.1968	244.1453
	C	2.078937	3.300198	-0.807656	259.8867	289.0741	312.3580
	C	-0.812378	2.272547	2.082588	321.3945	355.1364	398.1160
	C	2.889038	1.008826	-0.814613	413.2536	421.8580	437.9048
	C	-0.737193	3.597138	1.614133	461.4426	469.3160	487.8971
	C	3.013722	2.386696	-1.175951	504.3394	527.5012	540.9513
	C	1.535510	-0.884139	-0.031122	543.7829	557.2923	575.1948
	C	3.955126	0.111279	-1.097952	603.2412	619.6926	639.4037
	C	2.675318	-1.718873	-0.176408	651.5560	670.4451	689.3687
	C	3.887326	-1.189276	-0.698911	693.5248	699.0725	727.5423
	C	2.602435	-3.105051	0.165686	742.5410	757.7745	776.3708
	C	1.430510	-3.680131	0.543619	792.4470	798.9879	808.1281
	C	0.247601	-1.553412	0.123947	814.1490	833.6290	846.6723
	C	0.214849	-2.938890	0.470865	863.2206	870.0560	884.5947
	C	-0.981966	-0.933025	-0.187309	931.1144	933.6117	939.5142
	C	-2.200190	-1.592810	-0.056998	947.5286	960.9733	967.5818
	C	-2.215663	-2.935969	0.405575	971.0304	978.4382	981.7028
	C	-1.032966	-3.585575	0.646062	999.1281	1001.4455	1006.4965
	C	-3.416650	-0.937578	-0.391237	1055.7293	1086.6537	1090.2941
	C	-4.453026	-0.377463	-0.674038	1106.6385	1154.3657	1168.3529
	C	-5.682900	0.247108	-0.997212	1175.3655	1180.8827	1184.5360
	C	-5.810880	1.509650	-1.427392	1205.2491	1216.1444	1231.8450
	H	-0.096855	0.281882	1.913455	1240.4976	1248.3199	1273.9942
	H	0.287726	4.940983	0.300971	1287.7426	1304.7245	1319.6193
	H	2.167392	4.338580	-1.108543	1333.4302	1357.0456	1366.7506
	H	-1.482271	2.024503	2.897899	1373.4799	1399.3499	1411.2993
	H	-1.368067	4.364953	2.047218	1418.8389	1446.6678	1450.3102
	H	3.878756	2.685108	-1.758605	1465.7571	1472.5529	1505.2293
	H	4.844651	0.498137	-1.583204	1526.8105	1542.2656	1550.7922
	H	4.733106	-1.855825	-0.827927	1581.2101	1617.4498	1643.5007
	H	3.514447	-3.690522	0.118557	1648.6450	1651.9742	1660.3143
	H	1.389843	-4.726268	0.827008	1664.7524	2295.1020	3128.5819
	H	-0.990948	0.081059	-0.557008	3145.8330	3157.3620	3158.8273
	H	-3.164675	-3.443152	0.528020	3159.7988	3161.8970	3164.3797
	H	-1.036883	-4.628619	0.944459	3171.8590	3176.9135	3178.1596
	H	-6.573302	-0.366613	-0.879177	3180.4297	3186.5629	3193.5139
	H	-4.950084	2.154427	-1.558314	3217.1079	3226.3816	3235.5609
	H	-6.785954	1.921116	-1.657643			
	C	1.658595	1.304097	0.329499	-99.5335	9.5703	21.1817
	C	2.398590	2.442815	-0.113554	27.4561	56.5178	67.7300
	C	0.649703	1.527091	1.299819	75.3821	97.8485	121.8511
	C	2.056839	-0.025867	-0.116238	159.4042	179.9090	184.8910
	C	2.007621	3.739135	0.298405	227.7924	235.1465	247.4363
	C	3.583723	2.258318	-0.888697	279.5082	313.5575	344.5225
	C	0.316438	2.796545	1.719726	359.7155	399.8147	413.8999
	C	3.355005	-0.152489	-0.677118	420.0360	450.5638	469.8630
	C	0.975753	3.921129	1.189564	477.8146	495.7913	520.5907
	C	4.074328	1.009401	-1.098217	530.1052	542.3129	552.6778
	C	1.273602	-1.233294	0.053077	558.6100	569.1421	611.8657
	C	3.964400	-1.433052	-0.786658	628.5842	629.3833	652.2156
	C	1.964744	-2.473988	0.084818	674.6683	676.8402	690.6369
	C	3.324938	-2.543737	-0.325286	717.1748	718.4400	726.0682

	C	1.287489	-3.666429	0.488238	757.1387	770.8829	776.2334
	C	-0.044434	-3.666107	0.753812	778.2867	790.7064	810.2326
	C	-0.181478	-1.290876	0.095148	823.2487	839.5177	852.9400
	C	-0.828892	-2.499124	0.502548	859.8272	884.1923	885.5028
	C	-1.016921	-0.239535	-0.386963	894.2777	912.6536	938.8234
	C	-2.365665	-0.394356	-0.323257	945.1639	956.6959	962.9612
	C	-3.034800	-1.509630	0.164114	968.9964	976.2917	980.9810
	C	-2.243013	-2.568958	0.564229	985.1110	998.8768	1047.0333
	C	-3.918438	1.567440	-1.116966	1062.4715	1083.7919	1091.5400
	C	-5.114780	1.028487	-1.426929	1111.8893	1145.3565	1160.9348
	C	-6.173576	0.847700	-0.501942	1172.9262	1178.5187	1184.0434
	C	-7.093248	0.677209	0.260043	1201.4261	1215.4739	1229.0195
	H	0.140296	0.681073	1.737554	1233.2844	1244.4897	1271.7077
	H	2.566167	4.590507	-0.076459	1287.5289	1305.7273	1324.5513
	H	4.123414	3.133258	-1.234837	1345.2766	1359.6507	1374.3809
	H	-0.451924	2.925780	2.473595	1389.7507	1403.9951	1413.6653
	H	0.695921	4.918354	1.509609	1436.3302	1443.5354	1450.7278
	H	5.027794	0.866668	-1.595650	1467.1122	1498.8118	1513.4297
	H	4.969727	-1.497229	-1.188707	1536.8467	1549.1205	1583.4967
	H	3.820103	-3.508711	-0.320391	1604.5721	1612.9323	1621.2427
	H	1.868462	-4.578016	0.578614	1648.0907	1653.2162	1660.3113
	H	-0.544898	-4.570256	1.083258	2184.3285	3140.2614	3151.8006
	H	-0.573138	0.651762	-0.809308	3156.7419	3157.0639	3158.6739
	H	-4.116838	-1.559315	0.205555	3159.5162	3161.5229	3170.1941
	H	-2.701141	-3.491973	0.906737	3176.4953	3177.5894	3179.0786
	H	-3.168950	1.720343	-1.882185	3180.0218	3185.6156	3194.3252
	H	-3.717125	1.970992	-0.133294	3217.6430	3249.3469	3476.1790
	H	-5.297987	0.677893	-2.439265			
	H	-7.899022	0.537320	0.937870			
TS [i12]-[i13]	C	0.321081	-1.517726	0.647736	-189.3571	15.0460	19.7242
	C	1.090988	-2.682491	0.345602	30.7422	56.1041	65.8529
	C	0.771017	-0.706906	1.719459	74.4817	85.2165	108.0305
	C	-0.940892	-1.293110	-0.047879	122.9167	174.3345	183.2587
	C	2.326258	-2.898808	1.001711	228.5462	233.6156	246.2086
	C	0.564014	-3.668391	-0.543008	279.9677	312.7558	333.8629
	C	1.956740	-0.961812	2.373319	344.5873	399.8514	414.1597
	C	-1.504969	-2.405606	-0.726609	419.8936	450.5830	469.6726
	C	2.764629	-2.048882	1.991041	476.6530	493.4899	519.4376
	C	-0.709775	-3.561915	-1.001291	521.3472	541.4767	552.8732
	C	-1.702694	-0.060232	-0.022017	560.6054	569.2562	612.2262
	C	-2.876416	-2.393647	-1.102992	628.9859	650.9762	653.2649
	C	-3.100996	-0.139798	-0.260006	662.6891	676.2881	691.5334
	C	-3.669360	-1.332220	-0.787127	698.0015	719.1313	729.2362
	C	-3.940922	0.990123	-0.011602	756.7135	768.1806	774.5137
	C	-3.420309	2.188071	0.359631	782.0787	790.5584	809.2294
	C	-1.136835	1.274277	0.131563	822.8428	838.3214	854.3376
	C	-2.005480	2.383722	0.378817	859.0774	883.5919	893.2292
	C	0.240285	1.566962	-0.089785	898.8275	928.2796	944.1339
	C	0.676939	2.845692	0.061606	946.3307	948.0306	961.4193
	C	-0.120670	3.932653	0.401904	967.6778	974.9522	980.0486
	C	-1.473010	3.685730	0.544400	997.4824	1001.7521	1045.6000
	C	3.161144	3.174132	-0.296384	1060.5429	1083.5111	1090.8506
	C	3.547044	2.338914	-1.088123	1112.1070	1145.8706	1160.8376
	C	3.893036	1.356151	-2.044915	1173.0811	1178.3248	1184.0714
	C	4.188733	0.080433	-1.753187	1201.6728	1215.1141	1229.4892
	H	0.162875	0.123841	2.045790	1233.9095	1244.6585	1271.4043
	H	2.906064	-3.776314	0.734588	1287.7225	1316.2444	1324.9531
	H	1.168929	-4.537723	-0.777636	1345.2580	1359.4720	1373.9798
	H	2.262242	-0.323512	3.194500	1389.7723	1403.6358	1413.5125
	H	3.704435	-2.234845	2.498588	1442.0781	1443.8854	1450.6788
	H	-1.152750	-4.356808	-1.591959	1467.1485	1498.3420	1512.9758
	H	-3.288780	-3.269850	-1.591569	1536.6896	1548.6220	1582.8609
	H	-4.734964	-1.354880	-0.988187	1610.4356	1621.1885	1641.0399
	H	-5.012260	0.865159	-0.127188	1647.7458	1653.6694	1660.7286
	H	-4.067049	3.033249	0.569464	2122.2438	3133.6304	3147.1536
	H	0.921877	0.784860	-0.393962	3147.9746	3156.0823	3157.7074
	H	0.280487	4.933427	0.521470	3158.5625	3160.8892	3167.2123
	H	-2.157158	4.502184	0.755739	3170.7449	3175.9037	3177.0360
	H	3.076643	3.961482	0.412201	3179.5213	3185.2629	3202.1726
H	3.914190	1.687960	-3.080357	3219.4532	3238.1578	3459.7009	

	H	4.171846	-0.289394	-0.735073			
	H	4.445900	-0.620720	-2.537576			
TS [i14]-p6	C	0.722823	1.577115	0.472776			
	C	0.795536	2.951986	0.093290	-539.1572	25.5498	47.5163
	C	-0.174744	1.242360	1.517798	59.5891	71.4400	84.5658
	C	1.651327	0.621033	-0.120189	98.1990	119.8903	143.3446
	C	-0.117790	3.882738	0.643669	158.7332	193.3354	222.2697
	C	1.847959	3.394657	-0.764899	245.6846	253.0521	280.4496
	C	-1.025674	2.175880	2.069051	308.4916	331.1956	342.4515
	C	2.795794	1.156429	-0.768951	352.0001	363.0152	414.3903
	C	-1.025951	3.504698	1.605130	417.5211	421.5785	441.4407
	C	2.843194	2.541914	-1.120038	465.6687	471.1375	482.9344
	C	1.543846	-0.820146	-0.022576	496.6148	514.5628	540.8309
	C	3.917812	0.326166	-1.040410	543.1087	557.2165	574.6945
	C	2.732817	-1.584893	-0.156517	602.5239	617.9100	621.1142
	C	3.919917	-0.979908	-0.653373	641.2161	670.1238	677.5085
	C	2.736220	-2.977050	0.170740	689.2678	692.6609	721.6563
	C	1.594417	-3.623705	0.523091	736.2996	758.5558	772.3756
	C	0.294688	-1.564237	0.108742	777.5211	794.5887	798.7112
	C	0.338581	-2.953073	0.440036	812.6408	831.0059	843.2708
	C	-0.964853	-1.012125	-0.212291	854.2602	858.1056	866.9538
	C	-2.147935	-1.729940	-0.100823	885.4714	891.0823	924.5365
	C	-2.083999	-3.077262	0.334952	947.4300	960.8958	966.8432
	C	-0.872659	-3.670147	0.583842	970.6715	978.0993	982.0079
	C	-3.460864	-1.164822	-0.440368	988.2105	997.0871	1000.9152
	C	-3.723825	0.127529	-0.775376	1041.4490	1055.7893	1087.5275
	C	-4.993116	0.581130	-1.193132	1095.4983	1154.2127	1169.2601
	C	-6.067113	0.999585	-1.551289	1176.4166	1181.9307	1184.4674
	H	-0.181844	0.235103	1.908054	1198.0852	1205.9951	1220.5315
	H	-0.063233	4.915497	0.315555	1231.7470	1241.9335	1250.8683
	H	1.878044	4.438150	-1.059383	1287.2802	1294.4404	1310.0774
	H	-1.691515	1.883367	2.872838	1315.7175	1343.5504	1358.7295
	H	-1.711683	4.229544	2.028603	1368.9194	1374.4680	1400.2182
	H	3.698774	2.895919	-1.685240	1413.7318	1429.0679	1449.4092
	H	4.790919	0.768963	-1.507260	1464.7286	1471.5142	1509.6997
	H	4.805552	-1.594280	-0.773596	1526.3227	1545.7688	1550.9369
	H	3.681780	-3.507346	0.132916	1584.2133	1607.3113	1621.4453
	H	1.610347	-4.673662	0.794583	1647.7738	1651.2380	1652.8355
H	-1.000552	-0.000329	-0.586738	1660.4430	2180.5073	3148.4134	
H	-3.002303	-3.643892	0.444088	3157.8947	3158.2180	3159.2355	
H	-0.824848	-4.716922	0.864722	3160.4307	3161.2472	3162.4691	
H	-4.221552	-1.141941	1.518821	3172.7595	3176.9781	3177.7613	
H	-4.264677	-1.885177	-0.557194	3179.0712	3180.7550	3187.4151	
H	-2.946652	0.882280	-0.700053	3217.1813	3221.4432	3476.5979	
H	-7.014995	1.359240	-1.868015				
TS [i14]-[i16]	C	-1.447666	-0.637743	-0.637729	-1692.2185	28.9924	50.4097
	C	-2.827722	-0.795793	-0.307400	57.4317	75.6100	85.5581
	C	-1.133129	0.238332	-1.705986	124.7079	130.5515	150.8512
	C	-0.456913	-1.478855	0.018089	196.6326	212.7793	233.6868
	C	-3.797187	0.026283	-0.929132	246.3572	267.8326	300.3708
	C	-3.227904	-1.849988	0.569593	316.8004	367.9337	379.5467
	C	-2.102857	0.992316	-2.332105	416.1375	419.4595	424.0605
	C	-0.931428	-2.637887	0.684692	441.2065	471.6773	476.9401
	C	-3.445669	0.916729	-1.917453	486.5604	511.9453	528.6363
	C	-2.322663	-2.772626	0.987067	537.1622	541.0674	553.8014
	C	0.972182	-1.265997	-0.031581	574.9314	583.2941	616.1366
	C	-0.029071	-3.683377	1.026130	617.2777	643.5359	658.4074
	C	1.824756	-2.380131	0.184316	663.9168	687.3230	697.8685
	C	1.290243	-3.594680	0.697089	720.2742	725.6609	755.5727
	C	3.228087	-2.273233	-0.067001	759.9481	777.3138	783.4713
	C	3.796842	-1.090667	-0.420891	807.2240	810.4220	831.7650
	C	1.610749	0.031851	-0.181069	839.0388	847.1132	856.0496
	C	3.022399	0.108571	-0.427544	861.0768	881.1984	882.8858
	C	0.988369	1.270913	0.032442	939.3573	948.6150	957.0663
	C	1.593999	2.497367	-0.058049	962.1531	966.9837	974.5209
	C	2.957029	2.551639	-0.419419	979.9362	994.3726	996.6950
	C	3.647297	1.371935	-0.585923	1017.7611	1056.4698	1074.1360
	C	0.696286	3.658381	0.318388	1086.1096	1103.9341	1147.4094
	C	-1.246118	3.255144	1.917842	1166.2108	1173.3153	1178.5159
C	-1.714563	3.423132	3.017903	1183.9466	1185.3180	1201.6878	

	C	-0.676776	3.023784	0.632379	1208.0986	1220.7441	1232.0945
	H	-0.115148	0.295371	-2.061897	1240.9955	1247.4191	1281.9672
	H	-4.836002	-0.088363	-0.637750	1288.4151	1301.6411	1336.0979
	H	-4.277128	-1.944326	0.828030	1347.9589	1361.1985	1361.8462
	H	-1.828323	1.636426	-3.160160	1377.2626	1390.0468	1407.8364
	H	-4.200797	1.526655	-2.400275	1412.8626	1446.3041	1452.9526
	H	-2.638363	-3.632828	1.567859	1468.0361	1482.8665	1505.2858
	H	-0.422968	-4.573676	1.504423	1519.3517	1541.3614	1546.1210
	H	1.965056	-4.424242	0.878347	1576.5088	1616.3381	1640.3230
	H	3.834256	-3.167078	0.034978	1646.7533	1651.0137	1659.7077
	H	4.859600	-1.026645	-0.629562	1671.3732	2165.8422	3030.7681
	H	3.463999	3.505836	-0.524400	3065.7991	3097.0873	3152.1779
	H	4.709318	1.391514	-0.807069	3156.7375	3157.3584	3159.0660
	H	0.615205	4.392473	-0.490138	3160.9452	3168.2960	3171.3714
	H	1.089850	4.187523	1.190673	3175.7038	3177.0187	3179.4956
	H	-2.130572	3.574489	3.983252	3184.4782	3219.5335	3476.4468
	H	-0.295739	1.803963	0.511698			
	H	-1.403675	3.110502	-0.175901			
	C	1.818884	1.168543	0.273267			
	C	2.691120	2.179866	-0.232949	-1655.2200	26.1341	52.5355
	C	0.923515	1.545723	1.305519	60.2141	74.9373	94.4405
	C	1.979315	-0.208315	-0.179916	110.9155	140.5122	147.5169
	C	2.529920	3.522043	0.186460	191.6563	216.8240	234.9786
	C	3.779313	1.814746	-1.082784	257.2770	278.3148	295.2046
	C	0.815847	2.852431	1.729649	317.0400	342.7180	378.6877
	C	3.203097	-0.532698	-0.822916	407.0904	411.5354	422.4967
	C	1.600381	3.862080	1.141530	446.2938	450.6529	482.2419
	C	4.059653	0.505048	-1.307067	488.5747	506.8051	532.3491
	C	1.035411	-1.281807	0.058564	540.5209	543.6843	554.0202
	C	3.603883	-1.891064	-0.953463	582.2859	594.6529	613.4715
	C	1.535045	-2.611005	0.068130	623.1146	641.6906	658.0980
	C	2.837579	-2.888805	-0.431333	667.6593	687.1230	696.7768
	C	0.718484	-3.683869	0.542961	721.4312	738.0753	756.7234
	C	-0.574448	-3.479491	0.905483	759.6935	775.7834	790.3506
	C	-0.407682	-1.115402	0.196637	796.6444	813.0026	825.4090
	C	-1.190562	-2.210928	0.683710	834.3530	844.4603	853.6207
	C	-1.089884	0.044121	-0.256718	877.6225	879.0967	884.1753
	C	-2.458784	0.159523	-0.133468	913.7976	941.5871	953.4007
	C	-3.168662	-0.893905	0.452270	960.7104	967.9827	971.5998
	C	-2.596854	-2.063542	0.849061	975.7373	980.4103	997.7721
	C	-3.350060	1.297832	-0.591208	1024.4874	1053.5325	1073.9717
	C	-5.881408	1.052444	-0.840589	1080.1755	1095.6449	1154.0398
	C	-6.846928	1.067067	-1.564974	1169.2836	1177.0568	1181.8231
	C	-4.740050	0.993084	0.011483	1187.2279	1188.0568	1197.4121
	H	0.323546	0.787823	1.787813	1218.4750	1226.7789	1231.1748
	H	3.184363	4.277221	-0.236315	1244.1957	1259.1025	1278.7819
	H	4.420491	2.596233	-1.476165	1286.9056	1298.2792	1324.3810
	H	0.129984	3.099477	2.532223	1354.3729	1361.5987	1365.5384
	H	1.497530	4.891313	1.466028	1374.8420	1393.3403	1400.0091
	H	4.944590	0.217204	-1.864696	1412.7483	1442.5476	1450.7158
	H	4.558021	-2.109013	-1.420901	1468.0645	1481.6295	1505.1832
	H	3.180934	-3.917579	-0.442593	1511.2456	1542.8091	1546.9722
	H	1.161465	-4.671798	0.611268	1584.2403	1617.2604	1630.9708
	H	-1.179241	-4.292873	1.291576	1648.1889	1652.0570	1659.8803
	H	-0.527764	0.842373	-0.722456	1662.4621	2168.1979	3040.1269
	H	-3.172891	-2.894324	1.243833	3068.2480	3083.5981	3156.7588
	H	-3.411200	1.323278	-1.682818	3157.1940	3158.8487	3159.5124
	H	-2.978176	2.273838	-0.266773	3161.5798	3169.4356	3176.4705
	H	-7.696409	1.088752	-2.202210	3177.4425	3179.9238	3185.2711
	H	-4.908393	1.478017	0.975293	3197.3773	3216.8267	3475.5655
	H	-4.483601	-0.212259	0.362858			
	C	-1.183578	-1.472942	0.438658	-599.3401	27.7882	30.2147
	C	-1.534441	-2.793421	0.022360	57.6711	67.2817	76.0362
	C	-0.302136	-1.356801	1.542449	96.6985	112.0175	121.6982
	C	-1.839838	-0.328915	-0.183993	142.2646	166.0321	189.6268
	C	-0.888820	-3.909489	0.605637	231.2483	244.5477	258.4281
	C	-2.600429	-2.982101	-0.909123	297.8757	312.6084	328.6047
	C	0.282367	-2.461635	2.122341	343.9391	400.4962	408.6922
	C	-3.029444	-0.589959	-0.914674	422.1851	427.7096	457.6456
	C	0.016173	-3.752338	1.629472	464.3899	473.6567	489.0953

	C	-3.357648	-1.926205	-1.303674	499.7768	516.7890	540.9993
	C	-1.426948	1.052018	-0.040231	544.7508	557.4807	590.7034
	C	-3.922605	0.470773	-1.230416	603.9858	619.9789	637.3832
	C	-2.409382	2.061420	-0.222242	653.0087	670.0846	689.4427
	C	-3.665024	1.739570	-0.807225	693.4898	699.8088	727.9222
	C	-2.130084	3.414169	0.146199	742.9174	758.0875	776.6644
	C	-0.900031	3.788559	0.586293	792.8505	799.2622	809.2547
	C	-0.057490	1.502914	0.184082	814.5687	833.8229	846.5826
	C	0.182266	2.860862	0.555504	863.4233	870.3938	884.9556
	C	1.070306	0.694330	-0.082141	933.5533	934.8751	937.5291
	C	2.368365	1.149327	0.113551	947.6191	961.2698	968.0191
	C	2.580524	2.462728	0.605374	971.4715	978.8950	982.0685
	C	1.508373	3.294097	0.800423	999.9697	1000.4257	1001.9431
	C	3.475973	0.300617	-0.205637	1055.8500	1086.9815	1090.2385
	C	4.298790	-0.425596	-0.739193	1105.3968	1154.4370	1168.4203
	C	5.280137	-1.296667	-1.257459	1175.5629	1181.0644	1184.7351
	C	6.538143	-0.937148	-1.558356	1205.0978	1216.0266	1231.8664
	H	-0.094697	-0.380278	1.955065	1240.3684	1247.9452	1269.4642
	H	-1.150508	-4.900960	0.250918	1287.6337	1303.4072	1315.5501
	H	-2.841115	-3.989787	-1.230438	1334.4677	1356.9625	1366.2015
	H	0.945344	-2.332190	2.970064	1373.5633	1399.2325	1410.1028
	H	0.494262	-4.615963	2.077468	1418.1688	1445.2925	1449.8688
	H	-4.231479	-2.075603	-1.928897	1465.6609	1471.4430	1506.2686
	H	-4.839235	0.237231	-1.761093	1526.6444	1543.3925	1550.7459
	H	-4.385509	2.535180	-0.962688	1581.6985	1617.6103	1638.2470
	H	-2.932545	4.139928	0.068027	1648.2011	1650.2475	1652.6308
	H	-0.704684	4.811458	0.889296	1660.4216	2222.4119	3131.1882
	H	0.933338	-0.303915	-0.469101	3147.3865	3157.3960	3159.0286
	H	3.591596	2.804176	0.788062	3159.8916	3162.0518	3165.5632
	H	1.666647	4.318980	1.118864	3172.3685	3176.9897	3178.3663
	H	4.329930	0.310940	1.627648	3180.5375	3186.7558	3196.4641
	H	4.968092	-2.326915	-1.413293	3217.2846	3227.0391	3238.1904
	H	6.886652	0.078840	-1.417516			
	H	7.242796	-1.660121	-1.950266			
TS [i16]-[i17]	C	-1.571091	-0.415442	0.520257	-435.0030	46.2554	56.2006
	C	-2.833615	-0.992662	0.185494	66.1996	82.6780	102.2140
	C	-0.769009	-1.112665	1.456323	110.2426	143.0397	162.9964
	C	-1.228083	0.901540	-0.000656	202.9212	219.9274	241.0264
	C	-3.171551	-2.277612	0.671431	261.1287	302.2182	312.2198
	C	-3.782169	-0.234465	-0.566410	329.8725	356.5873	368.9893
	C	-1.141093	-2.344074	1.951558	411.0753	419.0159	428.0291
	C	-2.286016	1.680509	-0.541524	450.2861	472.3299	478.1204
	C	-2.337304	-2.953688	1.530913	487.6452	508.3625	532.0248
	C	-3.539247	1.069403	-0.859670	540.4222	551.6483	569.2784
	C	0.083432	1.507103	0.078470	588.1791	615.6706	636.6065
	C	-2.117959	3.079758	-0.732035	655.7577	667.5823	672.5187
	C	0.166266	2.924925	0.044918	686.0816	705.4852	725.0425
	C	-0.960257	3.693555	-0.357869	745.6588	754.2864	758.5070
	C	1.386430	3.584181	0.392489	776.0993	783.9338	798.4241
	C	2.508716	2.879691	0.694565	807.5163	817.4751	833.9596
	C	1.342701	0.775548	0.124339	839.8725	855.4589	864.2633
	C	2.536591	1.463785	0.519727	869.6005	880.6903	931.6007
	C	1.517381	-0.549820	-0.306158	941.6312	953.5199	960.1576
	C	2.685609	-1.265355	-0.240631	964.3464	973.0154	978.7960
	C	3.810907	-0.595559	0.310738	992.7147	993.6349	1008.8205
	C	3.741236	0.734086	0.650960	1026.7659	1057.3932	1081.5196
	C	2.891725	-2.666727	-0.799607	1101.2362	1148.9703	1166.2156
	C	0.645441	-2.648398	-1.764835	1170.6836	1179.0768	1180.6707
	C	0.169946	-1.530040	-1.906664	1184.3856	1200.5857	1207.2793
	C	1.613337	-3.491413	-1.064146	1214.8364	1229.9461	1237.7435
	H	0.140905	-0.658802	1.817457	1242.9839	1257.0897	1287.9213
	H	-4.123758	-2.707238	0.378131	1320.2196	1337.6802	1347.6999
	H	-4.727312	-0.696443	-0.831155	1360.8956	1368.6701	1374.1354
	H	-0.510751	-2.838534	2.682462	1388.0539	1394.6403	1409.4132
	H	-2.614569	-3.930915	1.909906	1446.2075	1452.3528	1465.6317
	H	-4.296315	1.677741	-1.343224	1472.1537	1478.5209	1493.7792
	H	-2.951087	3.654965	-1.121385	1518.0032	1534.7343	1546.7904
	H	-0.861191	4.772430	-0.410523	1572.4746	1613.0070	1640.5612
H	1.389356	4.668515	0.425228	1648.1959	1649.6476	1659.7923	
H	3.418188	3.386307	1.000340	2041.6093	3010.2538	3024.6911	

	H	4.749983	-1.132438	0.411737	3049.3493	3060.6693	3143.3101
	H	4.627309	1.253925	0.999576	3155.6084	3156.1032	3157.8829
	H	3.537716	-3.230726	-0.118625	3160.1073	3167.1823	3170.0410
	H	3.445722	-2.574661	-1.741845	3174.8354	3175.9574	3178.8122
	H	-0.434228	-0.727401	-2.261695	3183.5907	3228.2895	3428.0583
	H	1.167166	-3.820745	-0.119180			
	H	1.868901	-4.392948	-1.629073			
TS [i15]-[i18]	C	-1.697396	-1.102844	0.297213			
	C	-2.673017	-2.063262	-0.110233	-366.8353	36.8712	49.9185
	C	-0.674096	-1.552457	1.169172	67.5202	78.9808	103.4421
	C	-1.871126	0.296870	-0.073636	122.6265	140.8533	165.6135
	C	-2.503085	-3.426552	0.230273	203.9066	213.7377	251.9188
	C	-3.860332	-1.627252	-0.773300	269.2020	291.3032	320.8199
	C	-0.555615	-2.878725	1.524445	343.7019	351.9093	378.0636
	C	-3.163747	0.687590	-0.512767	407.9630	416.7281	421.2364
	C	-1.456708	-3.836731	1.023260	445.8385	469.9097	482.8199
	C	-4.120821	-0.300674	-0.902921	495.0939	504.7419	530.7147
	C	-0.862155	1.328316	0.062431	541.7384	554.0356	559.4362
	C	-3.528465	2.062374	-0.528675	611.5673	621.2849	635.0547
	C	-1.305011	2.671268	0.199407	656.6299	660.4713	679.3394
	C	-2.655978	3.011192	-0.088448	691.1854	707.0508	725.7381
	C	-0.386780	3.695638	0.586200	739.6122	746.3209	757.7661
	C	0.938023	3.434950	0.741522	775.2176	789.2161	797.1932
	C	0.577266	1.112656	-0.019075	811.7493	816.2252	834.5061
	C	1.462358	2.157786	0.382730	850.9461	854.8663	865.3938
	C	1.149487	-0.044840	-0.607832	871.4446	884.0352	916.9674
	C	2.517423	-0.234633	-0.715224	923.9892	944.8495	957.3606
	C	3.337541	0.779327	-0.198025	962.5911	967.4708	974.0331
	C	2.868421	1.939508	0.331565	979.8474	995.6388	998.2870
	C	3.092362	-1.453991	-1.405267	1029.3597	1053.8254	1080.7710
	C	5.141774	-1.254498	-0.075288	1095.6282	1155.3884	1169.0903
	C	5.481642	-0.116386	0.206080	1176.6234	1183.3206	1189.2409
	C	4.149388	-2.213081	-0.553125	1193.4688	1197.2177	1211.7714
	H	0.019747	-0.835544	1.583415	1222.3313	1230.0509	1235.2071
	H	-3.241564	-4.141441	-0.117589	1245.3126	1280.6665	1286.9843
	H	-4.582054	-2.370101	-1.095715	1318.9997	1325.1921	1349.5385
	H	0.230371	-3.181100	2.207441	1358.0510	1367.4196	1375.5853
	H	-1.347378	-4.881457	1.291415	1391.6870	1399.8780	1411.4621
	H	-5.067121	0.038965	-1.310563	1439.8747	1449.8184	1467.6874
	H	-4.532600	2.330513	-0.838840	1476.2875	1482.3545	1495.6333
	H	-2.958293	4.049792	-0.007990	1511.0887	1539.5455	1546.1102
	H	-0.776778	4.693635	0.756564	1580.1023	1609.8606	1626.2706
	H	1.624437	4.211714	1.061106	1647.9921	1651.0332	1659.6006
H	0.493662	-0.801135	-1.018386	2066.6298	3025.4156	3028.2429	
H	3.532111	2.724846	0.682236	3061.2784	3080.7125	3141.7438	
H	3.579206	-1.142911	-2.335765	3156.2776	3156.9892	3158.5148	
H	2.288036	-2.143828	-1.672412	3160.7014	3168.5915	3175.5068	
H	6.054454	0.722813	0.525425	3176.4960	3179.2298	3184.5267	
H	4.605942	-3.003883	-1.156137	3192.5554	3216.7238	3435.2484	
H	3.669722	-2.700186	0.302881				
TS [i17]-[i19]	C	-1.570244	-0.503393	0.483153	-1519.9364	50.0908	63.4318
	C	-2.821911	-1.117543	0.179144	69.3598	101.2460	108.0727
	C	-0.727532	-1.170034	1.405680	123.5587	147.2747	183.1096
	C	-1.273282	0.815953	-0.058859	228.1725	244.3324	251.1858
	C	-3.115120	-2.404380	0.687990	289.0916	313.7385	328.0982
	C	-3.802165	-0.395017	-0.567898	368.4357	406.5659	415.6282
	C	-1.054500	-2.405583	1.921914	423.4930	436.0561	461.1229
	C	-2.360120	1.560933	-0.585670	475.9511	489.6166	496.5382
	C	-2.245648	-3.048728	1.536790	517.6126	524.0567	539.6662
	C	-3.599757	0.911024	-0.880452	549.9420	567.6368	602.0319
	C	0.022623	1.461499	0.010010	607.0326	622.9443	655.7108
	C	-2.237007	2.965300	-0.773774	665.1860	671.7016	692.8763
	C	0.042651	2.884974	0.029501	721.9149	730.6867	739.5050
	C	-1.105487	3.616179	-0.380073	750.4592	756.0489	775.0074
	C	1.214142	3.576011	0.463758	777.7143	790.1036	804.2434
	C	2.330799	2.893033	0.829673	809.1136	838.6738	840.2723
	C	1.307487	0.784263	0.051209	843.2616	857.9481	872.2221
	C	2.423404	1.488012	0.591897	882.5647	925.1906	933.5361
	C	1.552584	-0.514849	-0.534545	946.7939	957.3416	964.0347
	C	2.788156	-1.159244	-0.296495	966.4279	972.6980	978.4716

	C	3.797352	-0.507781	0.424156	984.3500	992.1846	1043.9129
	C	3.639975	0.803674	0.818722	1057.6135	1081.0610	1101.6607
	C	3.087227	-2.492675	-0.960071	1132.0337	1165.5774	1169.6988
	C	0.660810	-2.545953	-1.696391	1177.7856	1183.9170	1187.0822
	C	0.653211	-1.140269	-1.463778	1192.3347	1204.7967	1217.9890
	C	1.820830	-3.235035	-1.311575	1224.7046	1232.9521	1240.0709
	H	0.183797	-0.690954	1.733032	1244.0410	1256.6926	1284.1222
	H	-4.060270	-2.863649	0.418089	1290.0983	1310.2362	1349.3634
	H	-4.737266	-0.886504	-0.813969	1354.9664	1359.7140	1368.8227
	H	-0.393591	-2.877086	2.640976	1375.6596	1389.0904	1403.0135
	H	-2.488741	-4.028742	1.931396	1406.7359	1434.7490	1442.3683
	H	-4.380298	1.492354	-1.359759	1450.7447	1456.7921	1465.9735
	H	-3.087616	3.514950	-1.162070	1502.9294	1519.5373	1541.0085
	H	-1.047616	4.698878	-0.410302	1545.6845	1571.7558	1596.3517
	H	1.177010	4.657946	0.532445	1620.3564	1647.8399	1648.2025
	H	3.195460	3.411172	1.230070	1658.6469	2118.8476	2956.6375
	H	4.739625	-1.017275	0.599064	3046.8645	3120.2505	3154.3907
	H	4.460306	1.338551	1.284930	3157.2169	3158.6518	3159.4256
	H	3.742307	-3.097859	-0.325608	3161.3778	3167.3945	3174.2536
	H	3.647257	-2.311022	-1.891781	3176.3223	3176.7369	3178.2432
	H	-0.075016	-0.527591	-1.980646	3179.9509	3184.4276	3214.4138
	H	0.695131	-3.214288	-0.597960			
	H	1.858637	-4.321098	-1.372011			
	C	-1.783916	-1.035462	0.296905			
	C	-2.817282	-1.924129	-0.131812	-1521.2506	42.6956	58.0571
	C	-0.813276	-1.556082	1.189618	68.7182	90.9441	116.3883
	C	-1.847911	0.370441	-0.079968	128.7121	152.9432	190.8712
	C	-2.752320	-3.295522	0.211653	210.1525	234.3569	274.3371
	C	-3.954560	-1.405176	-0.821931	285.2421	311.4835	329.5944
	C	-0.796569	-2.887262	1.545217	360.9042	383.7684	412.6974
	C	-3.096334	0.853100	-0.552964	423.1087	442.4422	453.6249
	C	-1.753684	-3.778536	1.025021	476.5516	495.1263	503.9725
	C	-4.114496	-0.063680	-0.962034	512.9793	523.5681	542.2436
	C	-0.768805	1.326805	0.078648	548.9809	557.1664	599.7178
	C	-3.357233	2.251070	-0.582373	613.1770	622.5776	642.0092
	C	-1.114351	2.702312	0.197212	672.8470	688.7167	698.0053
	C	-2.427903	3.137414	-0.125331	722.3073	727.9585	742.7443
	C	-0.129990	3.660310	0.594042	757.7634	760.5964	776.3594
	C	1.168704	3.305622	0.772097	782.9821	795.9562	801.3246
	C	0.645417	1.007057	0.029100	814.6656	826.7789	832.4992
	C	1.605349	1.987103	0.434422	845.0299	856.0511	884.4070
	C	1.151858	-0.194706	-0.542823	890.6109	913.2108	921.9007
	C	2.491335	-0.480109	-0.599246	936.9639	950.7735	961.4650
	C	3.447731	0.440951	-0.050745	968.2744	971.7818	975.7915
	C	2.974485	1.665977	0.425740	981.0634	997.9717	1048.4780
	C	3.019291	-1.707392	-1.320816	1056.3551	1077.9351	1098.6212
	C	5.261141	-1.275880	-0.174353	1145.4120	1168.6341	1170.7927
	C	4.833211	0.084433	-0.059983	1178.4562	1184.0164	1191.3283
	C	4.312337	-2.179512	-0.690395	1193.4203	1207.6731	1219.3627
	H	-0.080301	-0.889829	1.620717	1228.1061	1233.2843	1244.6585
	H	-3.532472	-3.956382	-0.151544	1249.4067	1286.8174	1289.9565
	H	-4.721064	-2.094743	-1.158876	1300.2692	1305.7420	1336.9496
	H	-0.047529	-3.245214	2.242577	1350.5375	1360.5964	1370.8538
	H	-1.724396	-4.828191	1.294371	1380.4036	1392.7167	1412.0501
	H	-5.023791	0.342197	-1.392490	1427.5991	1433.0397	1449.2169
	H	-4.331016	2.590925	-0.917867	1455.0135	1464.6775	1470.8867
	H	-2.655694	4.195724	-0.058613	1503.1611	1514.7013	1533.7446
	H	-0.449370	4.685014	0.751301	1549.1779	1580.0716	1613.7643
	H	1.904842	4.032219	1.098437	1618.1022	1647.6165	1649.5127
	H	0.455022	-0.894350	-0.984004	1658.7655	2127.2064	2967.5921
	H	3.686045	2.404175	0.782924	3069.6895	3119.2461	3145.8924
	H	3.231474	-1.443006	-2.368750	3156.7087	3157.3423	3159.3317
	H	2.269704	-2.502109	-1.343510	3160.0805	3162.4697	3169.8507
	H	5.575835	0.861486	0.094851	3177.6736	3177.9560	3180.4076
	H	4.547736	-3.241284	-0.736229	3185.8496	3198.8344	3216.6126
	H	4.601613	-2.071520	0.597295			
	C	1.572875	-0.609941	-0.498831	-623.7860	46.8322	66.8532
	C	2.791171	-1.296166	-0.207085	68.1359	102.8989	113.1261
	C	0.682751	-1.230351	-1.408466	129.8944	175.1962	192.3748
	C	1.349643	0.717634	0.058845	244.1086	246.7485	256.7996
TS [i18]-[i20]							
TS [i19]-p7							

	C	3.009807	-2.593546	-0.726591	279.5988	304.8027	322.3368
	C	3.812489	-0.638666	0.544538	345.7633	370.6656	407.9128
	C	0.934981	-2.480649	-1.930454	424.5212	431.2111	436.2572
	C	2.476578	1.390416	0.598701	453.4700	475.6359	489.5037
	C	2.095139	-3.186694	-1.565825	517.2626	523.4426	531.4742
	C	3.679769	0.670237	0.880389	531.9578	545.6008	568.4212
	C	0.091520	1.441421	-0.006336	578.6197	621.8181	634.0915
	C	2.438906	2.797445	0.809008	642.6622	669.8930	689.0278
	C	0.164591	2.865430	-0.009577	703.4587	707.6965	750.8421
	C	1.353508	3.520065	0.417661	752.6130	757.1422	759.1774
	C	-0.951574	3.637015	-0.439853	772.1545	785.9158	808.7951
	C	-2.107529	3.029797	-0.823525	813.8065	820.3117	839.2076
	C	-1.235237	0.852174	-0.066058	842.2761	843.9029	860.2230
	C	-2.290084	1.635044	-0.603755	884.8814	899.4712	915.1334
	C	-1.593180	-0.441491	0.499178	929.4717	957.6977	964.9454
	C	-2.873684	-0.999546	0.212674	968.7656	973.9185	979.4390
	C	-3.826061	-0.247234	-0.531471	982.1765	996.2496	999.6321
	C	-3.561846	1.042196	-0.872783	1001.3648	1053.4941	1062.8996
	C	-3.214334	-2.287212	0.721832	1066.2861	1112.8043	1133.9335
	C	-0.775407	-1.133808	1.425961	1160.9964	1165.5197	1176.6610
	C	-1.165482	-2.334921	1.987178	1178.3553	1184.7613	1185.7208
	C	-2.382622	-2.926777	1.633748	1204.8241	1211.3276	1227.5914
	H	-0.208002	-0.706085	-1.721223	1232.7248	1241.0851	1246.3280
	H	3.933351	-3.103121	-0.471915	1274.9796	1297.5850	1318.3607
	H	4.721491	-1.182847	0.777687	1350.9964	1358.2630	1370.1609
	H	0.231974	-2.918693	-2.629446	1379.6056	1384.7538	1391.3627
	H	2.278512	-4.177392	-1.965922	1419.2643	1445.0296	1449.1766
	H	4.490953	1.201678	1.366638	1460.7242	1468.8592	1505.9469
	H	3.320246	3.287827	1.207843	1515.2382	1536.3309	1547.3271
	H	1.360765	4.603826	0.460002	1554.4856	1582.1862	1610.0621
	H	-0.845751	4.715323	-0.489793	1623.4647	1638.6027	1648.6779
	H	-2.934439	3.606643	-1.223099	1655.2736	1660.6545	3156.4497
	H	-4.785297	-0.697827	-0.762207	3158.5913	3158.9457	3160.5277
	H	-4.318459	1.652136	-1.354734	3162.3374	3166.0309	3172.7283
	H	-2.844419	-3.394232	-0.864651	3174.1360	3176.2932	3177.6413
	H	-4.222828	-2.650543	0.561579	3179.1480	3180.8597	3186.9353
	H	0.162863	-0.696496	1.733472	3189.6267	3220.5486	3220.9422
	H	-0.522966	-2.815496	2.716032			
	H	-2.678119	-3.875929	2.065111			
	C	-1.836162	-1.007857	0.307970	-598.7187	43.8518	57.5766
	C	-2.885151	-1.869938	-0.133364	68.8191	95.1318	117.3405
	C	-0.904596	-1.545390	1.230430	143.3634	167.0285	197.8639
	C	-1.849078	0.397581	-0.088252	228.7999	246.3347	269.0642
	C	-2.871515	-3.237595	0.229528	283.1810	292.6615	328.4338
	C	-3.992343	-1.327115	-0.855737	336.6596	360.5951	396.1731
	C	-0.936887	-2.871687	1.604047	413.0157	415.6165	443.7356
	C	-3.075797	0.909249	-0.594276	453.6525	478.3589	498.7889
	C	-1.908068	-3.740212	1.073102	505.4622	521.4989	535.6151
	C	-4.111122	0.015520	-1.014439	536.9718	554.3449	565.7117
	C	-0.750153	1.322737	0.073672	591.4450	614.4992	635.2021
	C	-3.292818	2.310465	-0.657097	641.4508	650.2561	693.2117
	C	-1.051703	2.705408	0.151659	704.2529	715.2575	749.7561
	C	-2.341803	3.177284	-0.203325	756.1037	759.4680	771.1645
	C	-0.046842	3.644658	0.567845	782.8785	783.9031	798.1281
	C	1.229883	3.260589	0.801643	811.3637	814.9241	831.9746
	C	0.669114	0.957410	0.063642	842.6273	855.7271	870.7630
	C	1.649087	1.923067	0.497319	884.5049	900.1993	908.6295
	C	1.144001	-0.240241	-0.475339	925.4012	934.7521	951.0415
	C	2.502892	-0.573046	-0.490226	961.9197	968.6401	974.7951
	C	3.460666	0.341807	0.061281	978.0712	981.4743	996.7063
	C	3.000746	1.581405	0.522634	998.5856	1035.9102	1052.3186
	C	2.974932	-1.810732	-1.044143	1072.9419	1096.8906	1139.1305
	C	4.835990	-0.031923	0.090913	1162.1463	1165.9815	1175.7915
	C	4.309666	-2.156945	-0.940339	1181.9555	1183.9261	1191.4860
	C	5.244650	-1.252653	-0.385560	1210.3485	1211.9365	1230.0864
	H	-0.159056	-0.897830	1.667998	1241.2971	1249.9162	1287.0348
	H	-3.663034	-3.878825	-0.144134	1290.1010	1303.0652	1324.0269
	H	-4.770373	-1.999207	-1.201440	1355.0511	1360.6396	1366.2291
	H	-0.213490	-3.242623	2.321295	1372.7374	1398.4739	1406.9804
	H	-1.916963	-4.786767	1.355638	1418.5327	1442.0904	1448.4634
TS [i20]-p8							

	H	-4.998218	0.441966	-1.470555	1460.0322	1471.2746	1505.9541
	H	-4.248248	2.673728	-1.019739	1507.6880	1536.2877	1543.6282
	H	-2.536051	4.243576	-0.162867	1565.5156	1579.8847	1615.9314
	H	-0.345777	4.678679	0.703258	1617.0984	1648.1798	1652.9370
	H	1.972090	3.972546	1.146034	1656.8953	1661.8567	3155.7475
	H	0.447373	-0.943238	-0.910447	3157.3118	3158.7994	3159.6714
	H	3.719898	2.315531	0.872738	3160.9186	3162.0061	3170.5245
	H	2.967026	-1.342350	-3.005548	3170.6436	3176.8345	3177.9719
	H	2.245306	-2.540879	-1.373974	3179.4811	3180.2790	3185.8112
	H	5.555752	0.663641	0.509502	3190.7502	3205.1559	3218.4838
	H	4.646929	-3.117827	-1.311099			
	H	6.291307	-1.531182	-0.338191			
	C	1.718317	1.204758	0.330784			
	C	2.498060	2.285956	-0.182260	18.5644	21.7441	47.5315
	C	0.874063	1.484334	1.434502	67.6184	78.8273	101.4027
	C	1.923306	-0.139240	-0.196253	117.8817	141.3913	172.8350
	C	2.291390	3.597085	0.309055	196.3064	214.2211	243.4099
	C	3.545555	2.021600	-1.116241	256.7076	292.7446	318.3422
	C	0.722703	2.763077	1.925249	327.5799	375.9620	389.0037
	C	3.117040	-0.364149	-0.931504	410.2701	420.5195	426.9711
	C	1.409804	3.840909	1.336337	442.2997	457.7955	463.9847
	C	3.881514	0.741246	-1.419854	478.7043	493.1256	508.7364
	C	1.057441	-1.274917	0.050860	540.3914	543.4876	550.8212
	C	3.581639	-1.690294	-1.152153	559.2506	598.3144	615.0895
	C	1.627174	-2.573301	-0.037602	633.1441	640.2246	645.9400
	C	2.907122	-2.752960	-0.631587	668.7469	689.1185	694.0600
	C	0.901758	-3.712517	0.430716	721.0264	731.2292	757.1808
	C	-0.375881	-3.600003	0.878780	762.6572	777.2769	792.7445
	C	-0.378640	-1.201947	0.290464	801.5330	813.8115	829.5914
	C	-1.069204	-2.358460	0.759943	834.8040	846.8709	863.2342
	C	-1.164452	-0.070690	-0.046478	877.0300	883.9304	885.7651
	C	-2.528075	-0.024196	0.163156	926.8810	947.0425	960.3357
	C	-3.174771	-1.144312	0.734246	967.4709	970.7587	978.4761
	C	-2.460262	-2.283141	1.012753	981.4528	984.6069	998.4142
	C	-3.339809	1.199557	-0.228121	1025.6284	1055.3326	1087.3548
	C	-4.305954	0.920452	-1.349934	1093.4185	1142.6810	1153.5944
	C	-5.654854	1.154756	-1.269152	1167.7085	1175.2982	1180.8422
	C	-6.855435	1.366924	-1.186005	1182.9819	1185.9008	1199.6142
	H	0.349719	0.672865	1.917779	1209.3729	1227.1186	1234.2535
	H	2.873711	4.406576	-0.118693	1241.1049	1250.8322	1287.7022
	H	4.115372	2.855196	-1.512510	1296.7364	1299.9184	1340.0283
	H	0.077807	2.935201	2.779614	1358.4371	1369.7089	1375.0018
	H	1.271849	4.847471	1.714485	1398.1680	1400.3247	1412.8430
	H	4.741702	0.529515	-2.046091	1430.8884	1449.1141	1464.2688
	H	4.513249	-1.831923	-1.689246	1471.2431	1474.2025	1512.3107
	H	3.304376	-3.758752	-0.715171	1527.5407	1548.1180	1552.4661
	H	1.401321	-4.675404	0.420700	1586.5456	1621.4689	1648.0253
	H	-0.911261	-4.464385	1.256707	1652.7043	1655.2102	1661.2071
	H	-0.683369	0.784776	-0.499645	2013.3594	3005.2962	3062.5064
	H	-4.243779	-1.110783	0.915065	3150.6991	3156.7231	3157.1182
	H	-2.963415	-3.162213	1.402057	3158.7430	3159.4198	3161.3735
	H	-2.649677	1.996819	-0.531488	3169.8766	3175.7299	3176.6649
	H	-3.891771	1.574587	0.638608	3177.7267	3179.8488	3185.4443
	H	-3.903887	0.505515	-2.269445	3203.8604	3216.7819	3468.9873
	H	-7.899241	1.551776	-1.120926			
	C	1.677798	1.270550	0.306401	25.0480	41.0406	59.3529
	C	2.428221	2.383769	-0.181419	70.7390	76.2766	115.0370
	C	0.749120	1.524219	1.346784	122.3558	135.7618	168.5155
	C	1.990648	-0.069988	-0.174961	192.2120	218.6957	242.6439
	C	2.117851	3.690714	0.264271	255.8402	276.8330	313.5555
	C	3.547093	2.160789	-1.040333	328.0042	350.3126	379.7982
	C	0.495122	2.802042	1.795695	408.1772	423.8017	426.8716
	C	3.239705	-0.241199	-0.828419	459.7100	473.3184	484.3937
	C	1.158699	3.904874	1.226620	506.2451	522.2352	538.2843
	C	3.972081	0.895816	-1.292479	540.9276	551.4873	557.1143
	C	1.175013	-1.247857	0.042662	594.2526	604.2666	616.8746
	C	3.789775	-1.542996	-0.990060	639.2049	664.9306	688.5654
	C	1.819336	-2.513958	0.017854	694.9319	720.4186	734.3297
	C	3.142696	-2.632271	-0.490448	748.0767	756.4324	760.1998
	C	1.129368	-3.683086	0.464004	776.6048	791.0411	797.8879

	C	-0.178807	-3.634128	0.830480	810.9180	818.2998	823.7245
	C	-0.275430	-1.251509	0.192359	837.7384	849.3948	864.1960
	C	-0.929045	-2.436506	0.644589	878.2130	884.5224	928.4440
	C	-1.098241	-0.175479	-0.217227	930.1927	941.5232	948.3349
	C	-2.477766	-0.200417	-0.091519	960.4220	967.5422	971.5150
	C	-3.095754	-1.344942	0.470480	979.0958	981.7480	988.7504
	C	-2.336719	-2.433238	0.812464	999.0689	1054.8561	1082.4859
	C	-3.266300	0.958431	-0.553280	1087.7526	1097.1681	1152.3445
	C	-4.566951	1.088517	-0.503345	1168.3555	1175.1384	1181.0253
	C	-5.904152	1.257115	-0.455929	1184.1061	1191.0041	1201.3129
	C	-6.807124	0.898502	-1.455321	1209.8258	1228.6414	1234.2213
	H	0.239302	0.694796	1.814788	1240.4329	1250.3096	1286.7415
	H	2.681239	4.523058	-0.144569	1293.9507	1301.3722	1340.5629
	H	4.094444	3.017380	-1.418846	1358.7378	1370.8977	1374.4210
	H	-0.214123	2.954485	2.601324	1396.0523	1399.6912	1413.9850
	H	0.940448	4.909470	1.570648	1438.5321	1449.4010	1466.8504
	H	4.881207	0.720881	-1.857994	1472.5311	1490.5101	1511.9550
	H	4.760379	-1.641678	-1.464006	1527.1979	1547.0196	1551.9670
	H	3.599090	-3.615515	-0.527004	1585.3318	1620.1027	1647.9159
	H	1.680027	-4.616839	0.504541	1651.1186	1652.2339	1660.4443
	H	-0.688546	-4.520593	1.192383	1885.4394	3063.0762	3094.0679
	H	-0.640543	0.696159	-0.663564	3149.5883	3156.8853	3157.5945
	H	-4.172969	-1.363617	0.590431	3159.0946	3160.0745	3161.4995
	H	-2.812748	-3.332238	1.190299	3170.5365	3176.3224	3177.3468
	H	-2.680875	1.779769	-0.973421	3179.7775	3181.6437	3185.6929
	H	-6.306371	1.714031	0.449130	3205.3241	3217.1607	3250.4570
	H	-6.470191	0.441855	-2.377024			
	H	-7.867211	1.072006	-1.326652			
	C	0.939665	1.545147	0.461017	19.0671	27.6421	56.6705
	C	1.115046	2.885361	0.001335	66.3087	73.5630	88.2452
	C	0.009688	1.339601	1.511693	121.6370	141.5065	158.6671
	C	1.797667	0.492672	-0.062492	188.8673	200.2000	235.7800
	C	0.252098	3.905959	0.465173	259.4959	280.3347	313.4936
	C	2.221683	3.202665	-0.844374	325.9152	349.7671	373.4445
	C	-0.789939	2.362554	1.981502	413.4822	419.7080	428.7642
	C	2.985315	0.898356	-0.725608	440.4128	472.9397	475.6687
	C	-0.701106	3.650338	1.424873	484.6163	510.5167	536.0790
	C	3.156821	2.260018	-1.128360	540.8248	552.1992	554.8118
	C	1.541231	-0.926247	0.057598	602.3709	619.0935	635.0922
	C	4.012662	-0.046710	-0.995312	662.2082	663.2621	674.3707
	C	2.616147	-1.829536	-0.153573	685.2755	691.6559	718.0702
	C	3.863080	-1.354254	-0.644552	725.2123	756.0822	762.9177
	C	2.439776	-3.233107	0.057854	770.3582	775.4873	788.5539
	C	1.225345	-3.761789	0.359550	796.5067	812.9923	832.3905
	C	0.221131	-1.509319	0.246575	839.4448	843.2900	860.7661
	C	0.069671	-2.926976	0.408658	879.2365	882.5974	942.2142
	C	-0.981008	-0.807598	0.181402	952.7229	960.2516	965.1760
	C	-2.251195	-1.285567	0.311332	967.7752	974.0043	976.4487
	C	-2.355589	-2.688325	0.518095	981.1289	994.0255	1008.4973
	C	-1.226913	-3.474336	0.564649	1024.6539	1059.0139	1083.6104
	C	-3.477408	-0.408307	0.198225	1102.7684	1148.8925	1167.8327
	C	-5.154247	0.560950	-1.393699	1169.1044	1179.9244	1180.8542
	C	-6.145661	1.236224	-1.467940	1185.0414	1208.4659	1209.9092
	C	-3.951921	-0.257566	-1.270027	1229.5271	1236.4588	1242.7282
	H	-0.030199	0.380480	2.005244	1259.2743	1286.5477	1292.4279
	H	0.381935	4.909834	0.074593	1308.5643	1332.2435	1349.8092
	H	2.338117	4.223942	-1.190784	1360.1729	1365.7292	1377.6229
	H	-1.475497	2.172642	2.799601	1389.4969	1404.1325	1412.2271
	H	-1.346734	4.444501	1.782049	1448.0797	1454.9773	1467.8640
	H	4.048398	2.517612	-1.690080	1476.4381	1492.5214	1497.8667
	H	4.928565	0.301273	-1.460652	1519.4457	1534.9054	1547.5618
	H	4.666574	-2.066079	-0.799432	1573.9392	1615.7486	1644.6316
	H	3.306807	-3.876012	-0.050496	1649.9362	1653.3194	1661.5918
	H	1.106547	-4.829106	0.513586	2220.1610	3024.0322	3046.7062
	H	-3.338538	-3.135412	0.635667	3055.9272	3097.4701	3147.5533
	H	-1.318871	-4.545485	0.709066	3157.0061	3157.8538	3159.9368
	H	-3.262693	0.583940	0.599774	3161.4461	3170.5763	3171.9409
	H	-4.292203	-0.832099	0.791670	3176.0786	3177.4198	3179.9494
	H	-7.020640	1.833446	-1.544242	3186.1773	3220.7031	3478.2418
	H	-4.140760	-1.249055	-1.696076			

[i16]

	H	-3.143033	0.184329	-1.861047			
[i15]	C	1.442180	1.357275	0.405660			
	C	1.981075	2.591587	-0.069805	21.9435	32.2523	56.0146
	C	0.621980	1.413171	1.560436	67.0422	81.7585	84.9534
	C	1.861740	0.106454	-0.215764	120.4195	142.7838	156.0335
	C	1.564105	3.811993	0.513127	187.0635	209.0289	248.2902
	C	3.007187	2.579378	-1.062998	251.5574	292.9694	313.8944
	C	0.264897	2.612218	2.138110	327.5159	351.3713	378.9671
	C	3.034800	0.149178	-1.014810	408.7263	418.0485	422.5216
	C	0.709374	3.830070	1.590609	441.9664	453.9004	478.4107
	C	3.555755	1.403228	-1.462947	490.5324	502.9594	536.3314
	C	1.233479	-1.182682	-0.006716	541.8480	548.7233	559.5629
	C	3.722407	-1.052476	-1.341001	609.5358	616.7897	637.4633
	C	2.026680	-2.344647	-0.202815	659.1120	664.4920	675.4345
	C	3.283819	-2.249443	-0.861631	684.5810	692.1985	719.0526
	C	1.550721	-3.622603	0.224401	722.8492	757.4526	762.3802
	C	0.302148	-3.777273	0.737813	770.0163	774.9765	784.8922
	C	-0.177291	-1.391100	0.300112	796.0442	812.2274	831.6712
	C	-0.611878	-2.682495	0.728841	839.4828	851.1997	868.8885
	C	-1.166946	-0.402175	0.062530	878.6173	884.9297	913.2311
	C	-2.514514	-0.601739	0.328728	944.8819	957.4850	963.5839
	C	-2.838839	-1.853650	0.850398	968.4050	968.9038	975.6256
	C	-1.985656	-2.885688	1.049487	981.0527	999.0780	1016.3631
	C	-3.557938	0.451745	0.041425	1025.1967	1055.1799	1081.5388
	C	-5.520998	1.051433	-1.396036	1096.0170	1155.3826	1168.0847
	C	-6.353997	1.892778	-1.602142	1175.7707	1180.4595	1184.1006
	C	-4.496534	0.048357	-1.123005	1191.2969	1205.0376	1221.2466
	H	0.282909	0.493016	2.013649	1229.5457	1233.8662	1244.7771
	H	1.963710	4.738216	0.113514	1271.0579	1284.6157	1287.9877
	H	3.391758	3.525331	-1.428832	1307.3740	1324.4914	1353.9643
	H	-0.353789	2.613611	3.028379	1362.3952	1368.8892	1375.4227
	H	0.408969	4.770751	2.037776	1391.9428	1397.7210	1411.0746
	H	4.404915	1.390905	-2.137939	1438.7151	1450.0109	1467.4638
	H	4.633665	-0.987566	-1.925556	1476.6176	1491.7174	1497.8396
H	3.854061	-3.157220	-1.026247	1511.8964	1539.2451	1546.1422	
H	2.217644	-4.473165	0.131265	1578.1191	1611.0546	1630.8774	
H	-0.042144	-4.745297	1.084956	1648.2436	1652.0656	1659.9399	
H	-0.869745	0.548243	-0.360431	2220.9202	3023.0636	3043.4503	
H	-2.313422	-3.857437	1.404587	3052.9364	3092.5361	3157.2218	
H	-3.070479	1.398846	-0.199807	3157.6373	3159.3353	3160.1139	
H	-4.166169	0.622065	0.934564	3162.1637	3170.6298	3177.0109	
H	-7.094016	2.630851	-1.791252	3178.3267	3180.4405	3186.1395	
H	-4.974410	-0.907952	-0.884614	3194.8279	3216.2365	3478.1224	
H	-3.899998	-0.120554	-2.026052				
[i17]	C	1.565275	-0.566134	-0.478362	49.3213	66.5359	68.1985
	C	2.792393	-1.228429	-0.172419	102.1673	112.0989	125.2185
	C	0.700074	-1.198258	-1.403584	161.3587	177.1034	232.1915
	C	1.316302	0.762747	0.067262	247.1725	248.8901	286.5666
	C	3.039146	-2.522874	-0.686084	317.4315	325.5031	369.2263
	C	3.797047	-0.546558	0.580858	390.9293	403.6550	418.2041
	C	0.982932	-2.442680	-1.924366	424.5090	436.9447	473.5304
	C	2.431260	1.463705	0.601336	486.5786	498.6997	515.6295
	C	2.148082	-3.130649	-1.540250	516.8433	538.3626	545.9669
	C	3.643239	0.764768	0.898664	556.5992	575.2175	606.0625
	C	0.049095	1.457294	-0.003686	619.1287	652.2982	668.3422
	C	2.362469	2.869472	0.794722	684.9535	696.3837	720.5515
	C	0.085769	2.878615	-0.020264	735.9414	747.8877	755.8139
	C	1.257998	3.564146	0.397217	769.4824	777.9851	792.1887
	C	-1.050724	3.617819	-0.474701	807.7899	816.4752	832.6909
	C	-2.185452	2.980951	-0.861674	838.7363	841.7708	857.6704
	C	-1.267660	0.828704	-0.055646	860.2119	882.9630	896.1665
	C	-2.345289	1.580864	-0.620699	924.2941	932.3804	954.3605
	C	-1.583987	-0.439505	0.529057	960.0933	964.9058	972.9789
	C	-2.839709	-1.022031	0.309824	978.2047	983.2905	989.7943
	C	-3.816843	-0.331168	-0.424652	994.1461	1017.6462	1048.9525
	C	-3.592019	0.960965	-0.841955	1060.5514	1104.3537	1128.1135
	C	-3.198854	-2.338862	0.974190	1165.2045	1169.5850	1170.2242
	C	-0.896171	-2.415059	1.735730	1178.3321	1184.3105	1189.3497
	C	-0.670678	-1.143437	1.464047	1194.5555	1211.2601	1218.3621
	C	-1.981912	-3.263586	1.199014	1232.9309	1238.5705	1244.6936

	H	-0.194478	-0.687253	-1.727762	1248.4053	1274.8154	1296.7389
	H	3.967105	-3.017182	-0.417875	1324.7693	1334.1741	1340.8169
	H	4.712724	-1.073758	0.826444	1361.0835	1363.0613	1369.5949
	H	0.304701	-2.887930	-2.643805	1394.3878	1401.4721	1416.4453
	H	2.356088	-4.116931	-1.939463	1445.4803	1451.1416	1463.4553
	H	4.443831	1.313929	1.382907	1467.7335	1473.1562	1505.1742
	H	3.231481	3.384655	1.189499	1522.7505	1544.4115	1552.6969
	H	1.241836	4.648262	0.428568	1579.5698	1608.7297	1629.6841
	H	-0.966776	4.697023	-0.544850	1648.0388	1651.6112	1658.7614
	H	-3.021039	3.533519	-1.277620	1685.2286	2990.8265	2999.5997
	H	-4.780694	-0.798812	-0.598038	3056.5208	3059.0290	3154.7109
	H	-4.382998	1.531750	-1.316473	3156.1285	3157.9349	3158.8075
	H	-3.962917	-2.857500	0.387558	3160.9396	3167.7948	3173.6017
	H	-3.647503	-2.117197	1.952151	3175.9351	3176.3134	3177.7152
	H	0.152597	-0.594475	1.904293	3179.5922	3184.0022	3219.1510
	H	-1.654900	-3.723634	0.256423			
	H	-2.249759	-4.079382	1.876566			
	C	-1.784498	-1.031551	0.295926			
	C	-2.816968	-1.920161	-0.134374	44.1492	56.9291	68.7982
	C	-0.820106	-1.550396	1.196188	92.9950	113.7850	137.2951
	C	-1.844440	0.374257	-0.085550	159.1407	186.3721	211.7843
	C	-2.756466	-3.290353	0.215048	237.6924	271.2311	284.9515
	C	-3.950547	-1.402030	-0.831295	317.8953	322.1476	351.2333
	C	-0.807975	-2.880070	1.557914	381.4247	404.7585	413.5875
	C	-3.091409	0.856442	-0.563470	426.4264	442.2768	454.0517
	C	-1.763620	-3.771932	1.036240	482.1910	499.2879	503.0580
	C	-4.108401	-0.060736	-0.974764	534.6308	548.7411	553.1738
	C	-0.765644	1.329837	0.073931	558.8086	579.1108	615.0192
	C	-3.352270	2.254502	-0.597318	624.8443	645.7358	680.7356
	C	-1.110730	2.704212	0.187966	691.1391	700.8940	724.9613
	C	-2.424201	3.140322	-0.139480	742.6243	752.5393	758.0684
	C	-0.128431	3.661627	0.587835	770.9927	777.5869	794.9766
	C	1.169608	3.305400	0.775310	803.9407	813.8551	825.3888
	C	0.652671	1.009049	0.034495	837.0631	841.3315	856.3911
	C	1.606053	1.988035	0.442484	884.0734	885.0837	902.8125
	C	1.163331	-0.192701	-0.524677	920.8689	927.7560	933.3833
	C	2.507905	-0.475181	-0.578241	947.7641	961.0432	967.5568
	C	3.444855	0.457527	-0.040256	974.2494	976.8267	979.9914
	C	2.983306	1.667291	0.435317	997.6922	1023.2101	1050.6982
	C	3.034056	-1.712529	-1.278464	1069.6560	1094.1564	1138.8905
	C	5.203592	-1.166016	-0.267547	1167.0621	1171.1949	1176.4597
	C	4.874914	0.089050	-0.016822	1180.3296	1183.8853	1199.3394
	C	4.305746	-2.293121	-0.604159	1204.4143	1208.1494	1229.4887
	H	-0.087190	-0.884053	1.627134	1232.2708	1243.8926	1247.8645
	H	-3.535939	-3.951129	-0.149916	1255.7521	1287.6820	1296.7494
	H	-4.716306	-2.091684	-1.169885	1319.1004	1331.6240	1348.9427
	H	-0.063167	-3.236165	2.260787	1359.9200	1373.9554	1380.1555
	H	-1.737749	-4.820583	1.310004	1394.7088	1409.0560	1419.5320
	H	-5.015486	0.345129	-1.410026	1448.9219	1466.9029	1469.0566
	H	-4.324992	2.593633	-0.936729	1476.7326	1477.5618	1509.5999
	H	-2.650866	4.199092	-0.075023	1515.1870	1538.9341	1549.1923
	H	-0.447050	4.687432	0.739845	1585.0628	1620.0006	1647.1378
	H	1.904032	4.033062	1.103602	1648.8860	1653.3064	1660.3455
	H	0.471014	-0.904465	-0.952891	1683.1906	2997.5037	3006.6910
	H	3.689894	2.408908	0.795524	3055.3258	3072.3533	3142.7047
	H	3.297824	-1.438627	-2.308090	3154.3624	3156.5442	3157.9859
	H	2.258362	-2.480023	-1.339295	3158.8657	3160.9580	3169.1843
	H	5.604058	0.847367	0.254553	3175.9326	3176.9404	3179.4353
	H	4.783608	-3.012519	-1.275739	3184.8580	3200.9323	3217.1607
	H	4.047973	-2.840014	0.312730			
	C	1.569760	-0.595259	-0.505409	46.2990	63.2215	66.6462
	C	2.788998	-1.279095	-0.213661	86.5241	104.2199	121.4995
	C	0.690024	-1.207757	-1.430526	138.1493	183.2207	223.4701
	C	1.338841	0.728486	0.060581	244.6569	251.8560	282.8034
	C	3.016825	-2.569691	-0.746240	312.9048	325.9006	366.0078
	C	3.804433	-0.624014	0.548559	404.1768	422.9843	424.0273
	C	0.953360	-2.449238	-1.967936	434.7367	460.0315	477.6302
	C	2.462802	1.401808	0.608815	489.4122	507.0592	515.5024
	C	2.112882	-3.155777	-1.601850	522.0327	541.3322	546.6725
	C	3.666412	0.682364	0.891602	566.2261	600.1407	615.4045

	C	0.078549	1.444630	-0.000237	624.3829	654.7900	673.2687
	C	2.417569	2.805069	0.831232	674.4563	687.6369	701.3450
	C	0.143407	2.867349	0.011356	727.8417	746.5162	754.4347
	C	1.326314	3.524623	0.445522	757.7310	774.3489	777.2393
	C	-0.977194	3.638729	-0.421261	807.2204	812.0041	814.0326
	C	-2.124635	3.031638	-0.819825	838.3121	839.2981	840.9634
	C	-1.246623	0.844420	-0.073031	858.0740	883.5447	905.2268
	C	-2.305569	1.629613	-0.616139	923.9505	933.4776	953.9154
	C	-1.591204	-0.451673	0.478719	956.2665	959.8966	965.3317
	C	-2.854591	-1.014142	0.180038	967.7094	972.3049	978.1504
	C	-3.806374	-0.272170	-0.532631	993.0392	996.0644	1041.4543
	C	-3.562835	1.037524	-0.877709	1059.8726	1102.7761	1105.1016
	C	-3.224411	-2.407962	0.646479	1139.0918	1165.5101	1171.1588
	C	-0.752606	-1.135304	1.412555	1178.1603	1180.8653	1184.4442
	C	-1.119481	-2.375461	1.973084	1193.5495	1201.6696	1203.1722
	C	-2.273284	-3.013067	1.627939	1215.5573	1232.5320	1242.3591
	H	-0.200195	-0.682040	-1.742672	1245.4654	1257.9664	1290.6084
	H	3.940425	-3.078507	-0.490160	1292.4450	1316.6499	1356.0446
	H	4.714052	-1.167005	0.782144	1359.5752	1368.9341	1380.9766
	H	0.262375	-2.878923	-2.684475	1387.7093	1406.5923	1413.9793
	H	2.305356	-4.139790	-2.014185	1431.5337	1445.7053	1449.3096
	H	4.473825	1.212806	1.385296	1463.5770	1469.4938	1504.2699
	H	3.294625	3.297313	1.237200	1523.2788	1541.2336	1548.5808
	H	1.326942	4.608023	0.498516	1566.1411	1581.6745	1602.9056
	H	-0.873792	4.717696	-0.463498	1623.3931	1648.6380	1650.6607
	H	-2.951480	3.608292	-1.220134	1659.7037	2918.1960	2974.1926
	H	-4.771057	-0.719813	-0.751285	3151.0814	3155.1521	3155.6942
	H	-4.339168	1.641520	-1.334575	3157.7456	3158.6682	3160.9327
	H	-3.309713	-3.067780	-0.235140	3168.7334	3173.3500	3175.4346
	H	-4.239867	-2.394707	1.068723	3175.6543	3177.8097	3179.7236
	H	0.160087	-0.666867	1.746381	3184.4729	3219.0313	3229.0603
	H	-0.454209	-2.827386	2.701666			
	H	-2.526441	-3.976689	2.056038			
	C	-1.824295	-1.017210	0.302824	41.3997	56.0857	68.8713
	C	-2.861569	-1.896160	-0.135454	81.3298	112.0383	119.0113
	C	-0.885423	-1.537713	1.228939	147.4786	195.6168	204.6553
	C	-1.854877	0.383463	-0.099514	232.7509	272.7009	282.1595
	C	-2.828766	-3.262012	0.234018	310.5648	333.9787	358.3630
	C	-3.972942	-1.370933	-0.862528	388.7252	411.6738	424.2465
	C	-0.900368	-2.862295	1.608934	442.8505	455.9865	477.0495
	C	-3.084465	0.877985	-0.609425	488.9556	501.0285	515.8075
	C	-1.859302	-3.746946	1.080813	534.7916	549.4044	555.1081
	C	-4.107032	-0.029716	-1.028511	569.0543	605.5187	612.4927
	C	-0.764681	1.324628	0.069323	624.2770	646.0371	664.8515
	C	-3.322456	2.278780	-0.667323	676.3524	692.7580	702.5220
	C	-1.091650	2.705700	0.160100	725.6561	744.9889	757.4919
	C	-2.389662	3.156746	-0.200900	767.9664	775.8367	781.7707
	C	-0.102595	3.653818	0.571714	795.0521	802.6133	814.3965
	C	1.184375	3.281618	0.791482	830.9880	841.1276	854.5097
	C	0.647653	0.982354	0.060961	883.8904	887.8917	898.0834
	C	1.610816	1.952317	0.481630	906.1599	926.1305	943.5427
	C	1.152058	-0.232427	-0.471247	954.7902	959.5595	962.1722
	C	2.491205	-0.544179	-0.492536	967.3583	967.7256	974.0155
	C	3.443313	0.380501	0.047826	979.5037	998.4214	1048.3196
	C	2.974029	1.612832	0.504320	1060.8792	1086.9495	1103.6609
	C	2.960923	-1.854849	-1.097099	1151.2280	1168.8049	1172.3002
	C	4.831706	0.039252	0.073259	1175.5033	1183.4502	1188.5328
	C	4.432267	-2.109678	-0.976787	1195.1189	1205.2761	1209.0114
	C	5.286589	-1.194802	-0.424554	1227.5125	1232.4680	1244.6735
	H	-0.151205	-0.876222	1.665194	1256.0288	1287.9989	1298.2552
	H	-3.610902	-3.916170	-0.137145	1313.6065	1322.9012	1351.1490
	H	-4.742334	-2.053768	-1.206681	1359.9126	1371.6094	1382.1205
	H	-0.174741	-3.219593	2.330997	1396.3485	1412.5268	1422.1045
	H	-1.854492	-4.791998	1.369110	1445.1748	1447.6611	1450.3196
	H	-4.998761	0.383486	-1.487958	1462.8540	1472.1639	1509.0056
	H	-4.282203	2.628646	-1.031805	1519.9262	1537.5077	1547.5516
	H	-2.601633	4.219545	-0.154913	1563.2917	1581.2347	1615.0010
	H	-0.410179	4.685335	0.707130	1628.4351	1647.6706	1651.0866
	H	1.922285	4.001742	1.128429	1659.0218	2954.3213	2979.2551
	H	0.455172	-0.941273	-0.898230	3152.4589	3153.9668	3156.4061

[i20]

	H	3.687461	2.351423	0.857152	3157.7328	3158.7363	3160.8234
	H	2.675178	-1.887210	-2.160685	3169.2806	3170.5168	3175.8216
	H	2.403796	-2.687116	-0.642854	3176.8227	3179.2650	3181.4264
	H	5.536074	0.750384	0.489387	3184.9124	3194.8155	3216.8007
	H	4.810872	-3.051655	-1.358237			
	H	6.346503	-1.421998	-0.370468			
5_helicenyl	C	-1.581890	-0.372869	0.177977	65.3040	72.5384	90.7471
	C	-2.957272	-0.285639	-0.197950	120.1284	172.3097	177.5815
	C	-1.178361	-1.532164	0.886471	231.5048	245.1348	278.6399
	C	-0.703902	0.768253	-0.051702	312.7345	343.6403	399.4229
	C	-3.812709	-1.394930	0.002923	413.1155	419.6204	449.9144
	C	-3.480929	0.951013	-0.683520	469.9617	477.7598	496.8619
	C	-2.042067	-2.582438	1.108842	518.4395	537.8726	545.3093
	C	-1.328488	2.016701	-0.310827	552.2910	567.5281	611.6022
	C	-3.365315	-2.532895	0.632896	626.4803	650.8386	673.6535
	C	-2.711139	2.069719	-0.671585	691.4039	717.5980	727.5049
	C	0.741240	0.745909	0.054486	756.8321	763.7678	774.2370
	C	-0.592741	3.226229	-0.173811	782.4896	791.5643	809.3902
	C	1.405240	1.968473	0.341765	820.8017	838.1123	856.8251
	C	0.705311	3.202296	0.238141	859.9374	881.6039	884.6324
	C	2.790088	1.971592	0.695968	931.8493	944.8117	951.1480
	C	3.527891	0.831854	0.670488	962.5356	968.8668	976.1237
	C	1.584765	-0.412359	-0.208775	981.0937	998.6637	1047.8897
	C	2.967676	-0.377038	0.155299	1062.8282	1082.1904	1091.5193
	C	1.138526	-1.548923	-0.948087	1143.2076	1160.8101	1172.8456
	C	2.011652	-2.566668	-1.156112	1178.7325	1184.1668	1201.0184
	C	3.331979	-2.622481	-0.732626	1215.1176	1228.7572	1233.3866
	C	3.802338	-1.497484	-0.080979	1244.4467	1268.0070	1287.1121
	H	-0.173977	-1.589579	1.279841	1322.2534	1343.2164	1359.5375
	H	-4.845662	-1.315554	-0.319555	1374.4292	1389.3832	1403.1462
	H	-4.522198	0.995542	-0.984097	1414.4826	1442.4288	1450.6335
	H	-1.699083	-3.448193	1.663870	1467.1466	1496.8366	1513.7062
	H	-4.034204	-3.370654	0.793765	1536.2778	1549.3033	1582.9360
	H	-3.131745	3.032885	-0.940390	1610.4618	1621.5994	1648.3456
	H	1.243841	4.123143	0.433936	1653.5807	1660.5992	3153.3998
	H	3.240140	2.914194	0.988523	3157.3643	3159.0921	3159.9179
	H	4.571917	0.839701	0.964301	3161.9091	3171.0204	3176.8089
	H	0.133470	-1.580643	-1.345424	3177.9722	3179.7908	3180.5051
H	3.970161	-3.478193	-0.919630	3186.1317	3199.5361	3217.4037	
H	4.839841	-1.446831	0.235018				

Table S2.

Bimolecular reactions and degradation pathways incorporated into the astrochemical models.

R_1	R_2	P_1	P_2	α	β	γ	No.
C3H3	C3H3	C6H5	H	4.00E-10	0	0	1
C4H6	C2H	C6H6	H	4.00E-10	0	0	2
C2H4	C2H	C4H4	H	4.00E-10	0	0	3
C6H6	C	C6H5C	H	4.00E-10	0	0	4
C6H6	CH	C6H5CH	H	4.00E-10	0	0	5
C6H6	C2	C6H5C2	H	4.00E-10	0	0	6
C6H6	C2H	C6H5C2H	H	4.00E-10	0	0	7
C6H6	CN	C6H5CN	H	4.00E-10	0	0	8
C6H6	hv	C6H5	H	3.00E-09	0	3.1	9
C6H5	C4H4	C10H8	H	4.00E-10	0	0	10
C10H8	C	C10H7C	H	4.00E-10	0	0	11
C10H8	CH	C10H7CH	H	4.00E-10	0	0	12
C10H8	C2	C10H7C2	H	4.00E-10	0	0	13
C10H8	C2H	C10H7C2H	H	4.00E-10	0	0	14
C10H8	CN	C10H7CN	H	4.00E-10	0	0	15
C10H8	hv	C10H7	H	2.00E-09	0	3.1	16
C10H7	C4H4	C14H10	H	4.00E-10	0	0	17
C10H8	hv	C9H7C	H	2.00E-09	0	3.1	18
C9H7C	C4H4	C14H10	H	2.00E-10	0	0	19
C9H7C	C4H4	C13H10C	H	2.00E-10	0	0	20
C14H10	hv	C14H9	H	4.60E-09	0	3.1	21
C13H10C	hv	C13H9C	H	4.60E-09	0	3.1	22
C14H10	C	C14H9C	H	4.00E-10	0	0	23
C14H10	CH	C14H9CH	H	4.00E-10	0	0	24
C14H10	C2	C14H9C2	H	4.00E-10	0	0	25
C14H10	C2H	C14H9C2H	H	4.00E-10	0	0	26
C14H10	CN	C14H9CN	H	4.00E-10	0	0	27
C13H10C	C	C13H9CC	H	4.00E-10	0	0	28
C13H10C	CH	C13H9CCH	H	4.00E-10	0	0	29
C13H10C	C2	C13H9CC2	H	4.00E-10	0	0	30
C13H10C	C2H	C13H9CC2H	H	4.00E-10	0	0	31
C13H10C	CN	C13H9CCN	H	4.00E-10	0	0	32
C2	C4H6	C6H5	H	4.00E-10	0	0	33
C6H4CN	C4H4	C10H7CN	H	4.00E-10	0	0	34
C6H5CN	hv	C6H4CN	H	3.00E-09	0	3.1	35
C10H7CN	hv	C10H6CN	H	3.00E-09	0	3.1	36
C10H6CN	C4H4	C14H9CN	H	4.00E-10	0	0	37
C2H4	CH	CH2CCH2	H	4.00E-10	0	0	38
CH2CCH2	hv	C3H3	H	3.00E-09	0	3.1	39
C2H4	C	C3H3	H	4.00E-10	0	0	40
C2H6	hv	C2H4	H2	3.00E-09	0	3.1	41
C2H6	CH	C3H6	H	4.00E-10	0	0	42
C3H6	CH	C4H6	H	4.00E-10	0	0	43
C4H6	CH	C5H6	H	4.00E-10	0	0	44
C5H6	CN	C5H5CN	H	4.00E-10	0	0	45
C5H5CN	CH	C6H5CN	H	4.00E-10	0	0	46
C5H6	CH	C6H6	H	4.00E-10	0	0	47
C14H9	C4H4	C18H12	H	4.00E-10	0	0	48
C18H12	hv	C18H11	H	3.00E-09	0	3.1	49
C18H11	C4H4	C22H14	H	4.00E-10	0	0	50
C22H14	hv	C22H13	H	3.00E-09	0	3.1	51
C22H13	C4H4	C26H16	H	4.00E-10	0	0	52
C26H16	hv	C26H15	H	3.00E-09	0	3.1	53
C18H12	C	C18H11C	H	4.00E-10	0	0	54
C18H12	CH	C18H11CH	H	4.00E-10	0	0	55
C18H12	C2	C18H11C2	H	4.00E-10	0	0	56

C18H12	C2H	C18H11C2H	H	4.00E-10	0	0	57
C18H12	CN	C18H11CN	H	4.00E-10	0	0	58
C22H14	C	C22H13C	H	4.00E-10	0	0	59
C22H14	CH	C22H13CH	H	4.00E-10	0	0	60
C22H14	C2	C22H13C2	H	4.00E-10	0	0	61
C22H14	C2H	C22H13C2H	H	4.00E-10	0	0	62
C22H14	CN	C22H13CN	H	4.00E-10	0	0	63
C26H16	C	C26H15C	H	4.00E-10	0	0	64
C26H16	CH	C26H15CH	H	4.00E-10	0	0	65
C26H16	C2	C26H15C2	H	4.00E-10	0	0	66
C26H16	C2H	C26H15C2H	H	4.00E-10	0	0	67
C26H16	CN	C26H15CN	H	4.00E-10	0	0	68

Note: R1 and R2 are reactants, P1 and P2 are the products. Reaction rate coefficients and (preexponential) factors α (s^{-1}) are parameterized according to Section 2.1 of D. McElroy, C. Walsh, A. J. Markwick, M. A. Cordiner, K. Smith, T. J. Millar, The UMIST database for astrochemistry 2012, A&A, 550, A36 (2013). The in the table are given at 300 K.