

Supporting Information

An Unconventional Dark Radical Chemistry in Dense Molecular Cloud: Directed Gas-Phase Formation of Naphthyl Radicals

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Laboratory and center-of-mass frame

For a bimolecular reaction of $A + BC \rightarrow AB + C$ studied in our universal crossed molecular beam machine (Figure S2), in laboratory frame, the collision energy E_c , the center-of-mass angle Θ_{CM} , the center-of-mass velocity can be expressed as follows:

$$E_c = \frac{1}{2} \frac{m_A m_{BC}}{m_A + m_{BC}} (v_A^2 + v_{BC}^2)$$
$$\Theta_{CM} = \tan^{-1} \left(\frac{m_{BC} v_{BC}}{m_A v_A} \right)$$
$$|v_{CM}| = \frac{\sqrt{(m_A v_A)^2 + (m_{BC} v_{BC})^2}}{(m_A + m_{BC})}$$

In the center-of-mass frame, for the heavy product AB, the center-of-mass velocity u_{AB} is

$$u_{AB} = \sqrt{\frac{2m_C}{m_{AB}} \frac{E_c - \Delta_r G}{m_{AB} + m_C}}$$

where $\Delta_r G$ represents the reaction energy. Noted that the product number density is recorded in the LAB frame, and considering the conservation of the scattering flux I ($\text{m}^{-2}\text{s}^{-1}$),

$$I_{LAB} \Omega = I_{CM} \omega$$

where Ω and ω represent the laboratory solid angle and the corresponding CM solid angle, respectively (Figure S2). These details overall explain the experimental planning and the transformation from the LAB frame to the CM frame for interpretation.

Supplementary experimental results

For the carbon – indene reaction, it should be noted that the dicarbon (C_2) and tricarbon (C_3) were also generated in the primary beam. The experimental conditions are optimized to make sure that the concentration of the dicarbon is less than 5% compared to the atomic carbon. No signal was detected at higher m/z in the reaction. Tricarbon will not contribute to the signal because of the significant entrance barriers.^{1,2} In addition, our laboratory signal recorded at m/z 127 can only be fit with a single H loss channel instead of other routes involving C_2 or C_3 along with indene.

For the dicarbon – styrene reaction, since the atomic hydrogen can be eliminated from the vinyl moiety and/or the aromatic ring of the styrene, the reactions of dicarbon with D3- and D5-styrene were performed to trace the source. Signal was probed at m/z 130 ($C_{10}H_4D_3^+$) and 129 ($C_{10}H_3D_3^+/C_{10}H_5D_2^+$) in the C_2 - $C_6H_5C_2D_3$ reaction (reaction S1) with the determined ratio of $1: 1.22 \pm 0.03$ of 130 to 129 taking into consideration of the ^{13}C isotopic contribution and the difference of the recoil circles related to atomic hydrogen and deuterium loss. For the C_2 - $C_6D_5C_2H_3$ system (reaction S2) the ratio of 1 (132): 0.78 ± 0.02 (131) is calculated according to the same procedure. Meanwhile, the experimentally derived ratio of 127: 126 in the C_2 - C_8H_8 system is measured to be 1.00 (127): 0.62 ± 0.03 (126) and the relative ratios of 132: 130 using D5/D3-styrene are computed to be $1.28 \pm 0.05:1$ under the same experimental conditions of the secondary beam (pressure, pulse voltage, etc) and calibrated according to the intensity of the primary dicarbon beam.

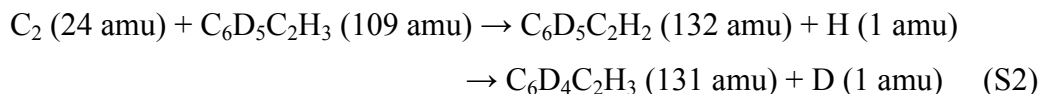
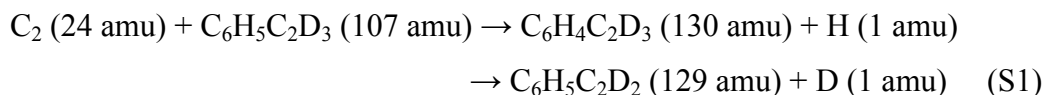


Table S1. Peak velocity (v_p) and speed ratios (S) of the atomic carbon (C ; 3P), dicarbon (C_2 ; $X^1\Sigma_g^+/a^3\Pi_u$), indene (C_9H_8 ; X^1A'), and styrene (C_8H_8 ; X^1A') beams along with the corresponding collision energy (E_c) and center-of-mass angle (θ_{CM}) for each reactive scattering experiment. The peak velocity and collision energy are measured in the laboratory frame.

beam	v_p (m s $^{-1}$)	S	E_c (kJ mol $^{-1}$)	θ_{CM} (deg)
C	2538 ± 46	2.8 ± 0.3		
C_9H_8	367 ± 6	15.2 ± 1.4	35.8 ± 1.2	54.4 ± 0.5
C_2	1408 ± 21	3.5 ± 0.4		
C_8H_8	372 ± 6	12.8 ± 0.6	20.6 ± 0.5	48.9 ± 0.4

Table S2. RRKM calculated product branching ratios (%) for various initial complexes for the triplet potential energy surface (PES) for the reaction of atomic carbon ($C, {}^3P$) with indene (C_9H_8).

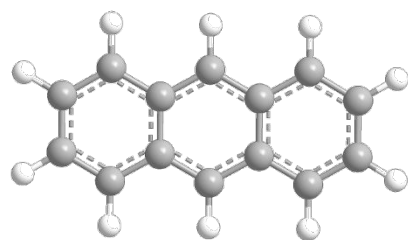
products	RRKM (%)		
	Initial complex		
	i1	i5	i7
p1 (2-naphthyl)	99.99	99.84	0.16
p2 (1-naphthyl)	0.01	0.01	0.00
p3	0.00	0.15	99.84

Table S3. RRKM calculated product branching ratios (%) for various initial complexes for the singlet potential energy surface (PES) for the reaction of dicarbon ($C_2, X^1\Sigma_g^+$) with styrene (C_8H_8, X^1A').

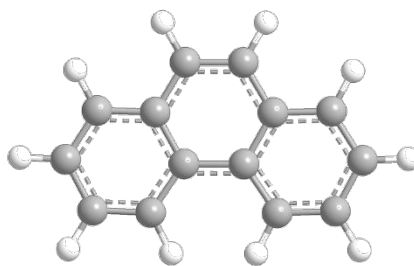
products	RRKM (%)		
	Initial complex		
	i1'	i3'	i2'
p1 (2-naphthyl)	67.34	0.45	94.00
p2 (1-naphthyl)	32.31	99.55	5.94
p5	0.00	0.00	0.00
p6	0.01	0.00	0.00
p7	0.34	0.00	0.06

Table S4. RRKM calculated product branching ratios (%) for the triplet potential energy surface (PES) for the reaction of dicarbon ($C_2, a^3\Pi_u$) with styrene (C_8H_8, X^1A').

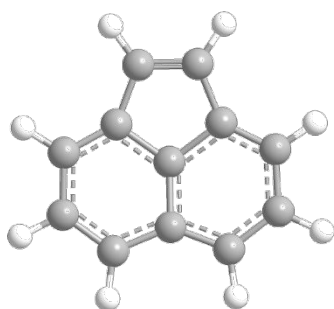
Ec (kJ mol ⁻¹)	p1 (2-naphthyl)	p2 (1-naphthyl)	p8
21	97.65%	2.35%	0%



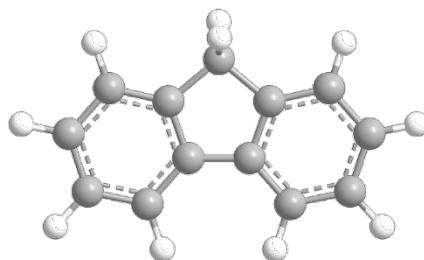
$C_{14}H_{10}$
anthracene



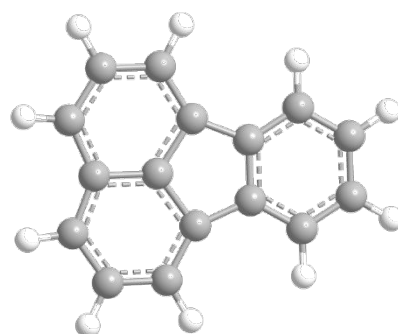
$C_{14}H_{10}$
phenanthrene



$C_{12}H_8$
acenaphthylene



$C_{13}H_{10}$
fluorene



$C_{16}H_{10}$
fluoranthene

Figure S1. Structures of anthracene ($C_{14}H_{10}$), phenanthrene ($C_{14}H_{10}$), acenaphthylene ($C_{12}H_8$), fluorene ($C_{13}H_{10}$), and fluoranthene ($C_{16}H_{10}$).

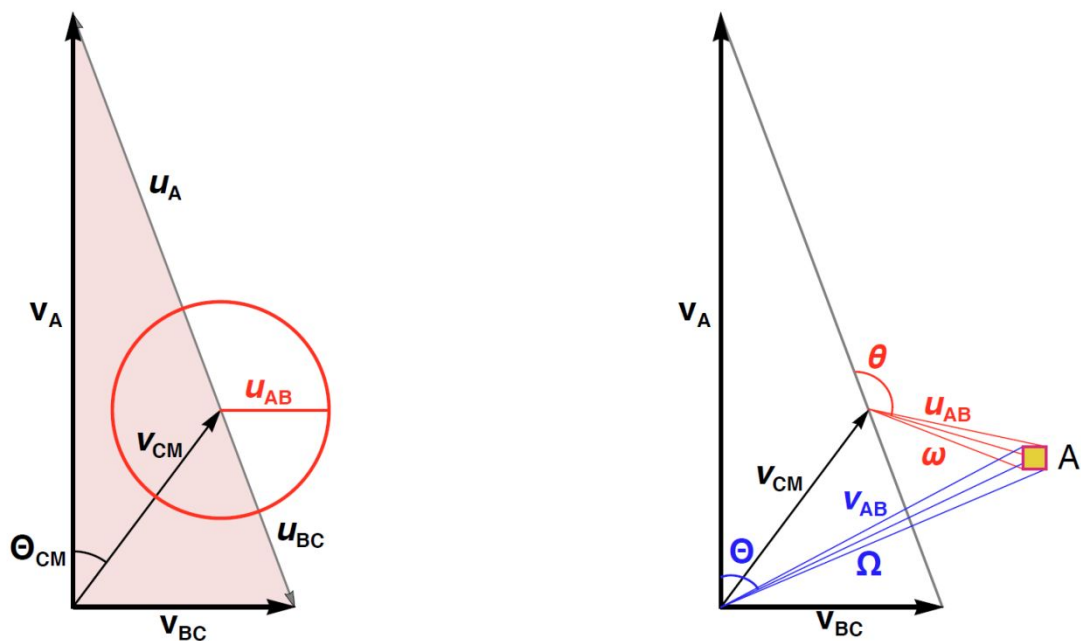


Figure S2. Newton diagram of a bimolecular reaction connecting the laboratory and center-of-mass frames.

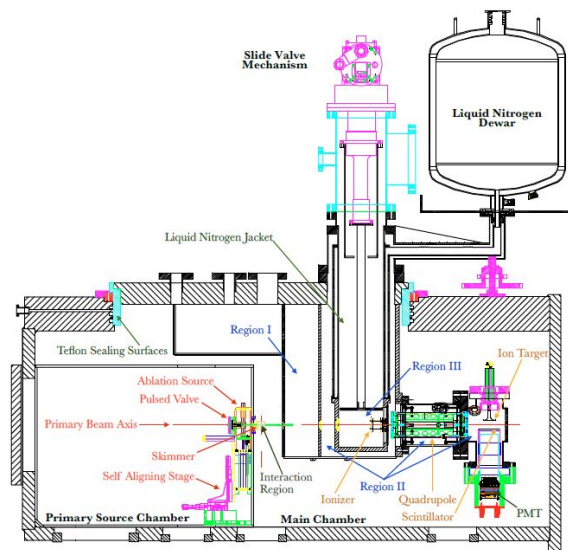
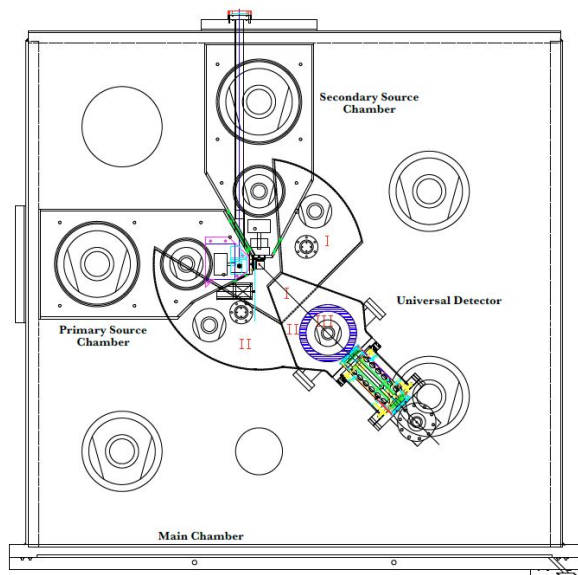


Figure S3. Cross sections of the CMB machine.

ω B97X-D/6-311G** / CCSD(T)-F12b/cc-pVTZ-F12

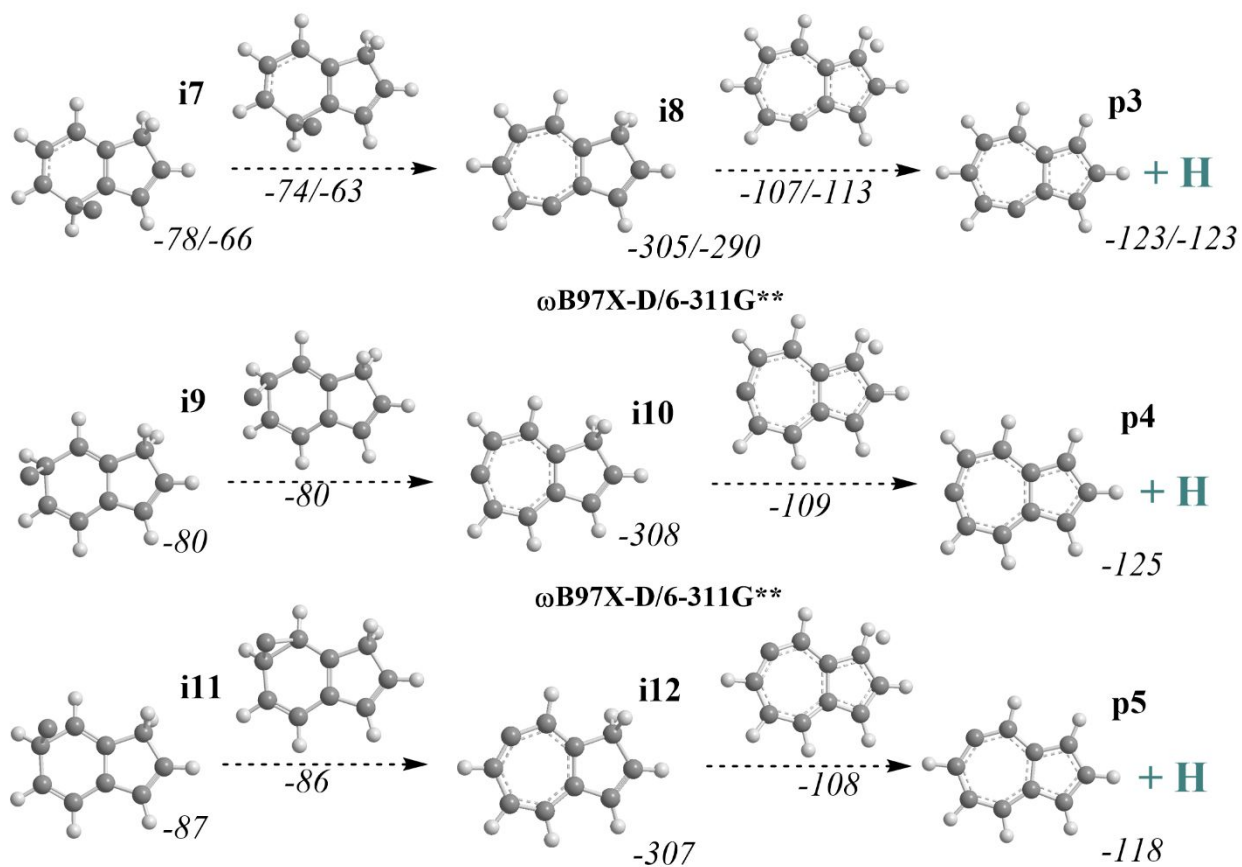
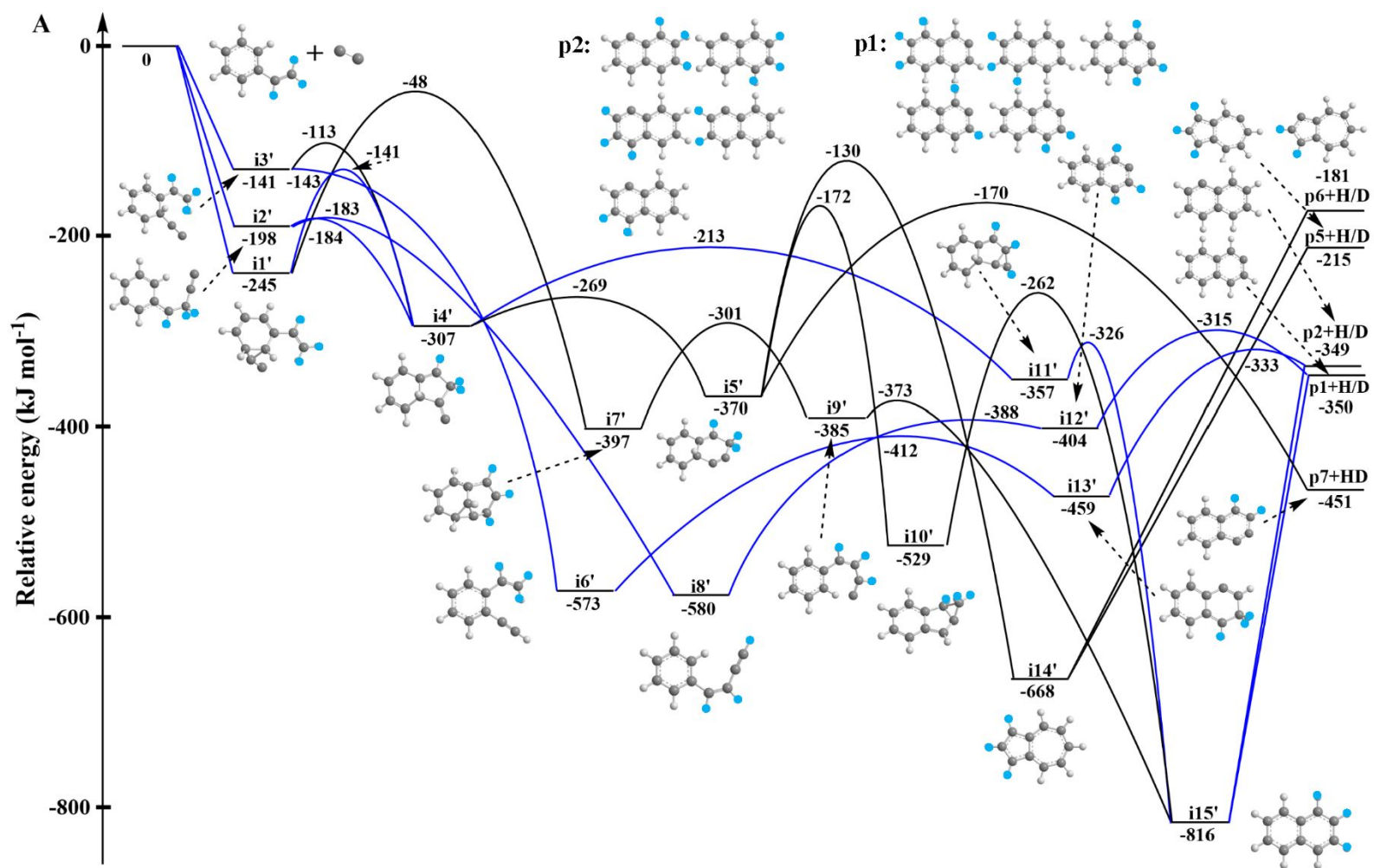


Figure S4. Additional pathways lead to the formation of **p3-p5** with fused five- and seven-membered rings in the C-C₉H₈ reaction.



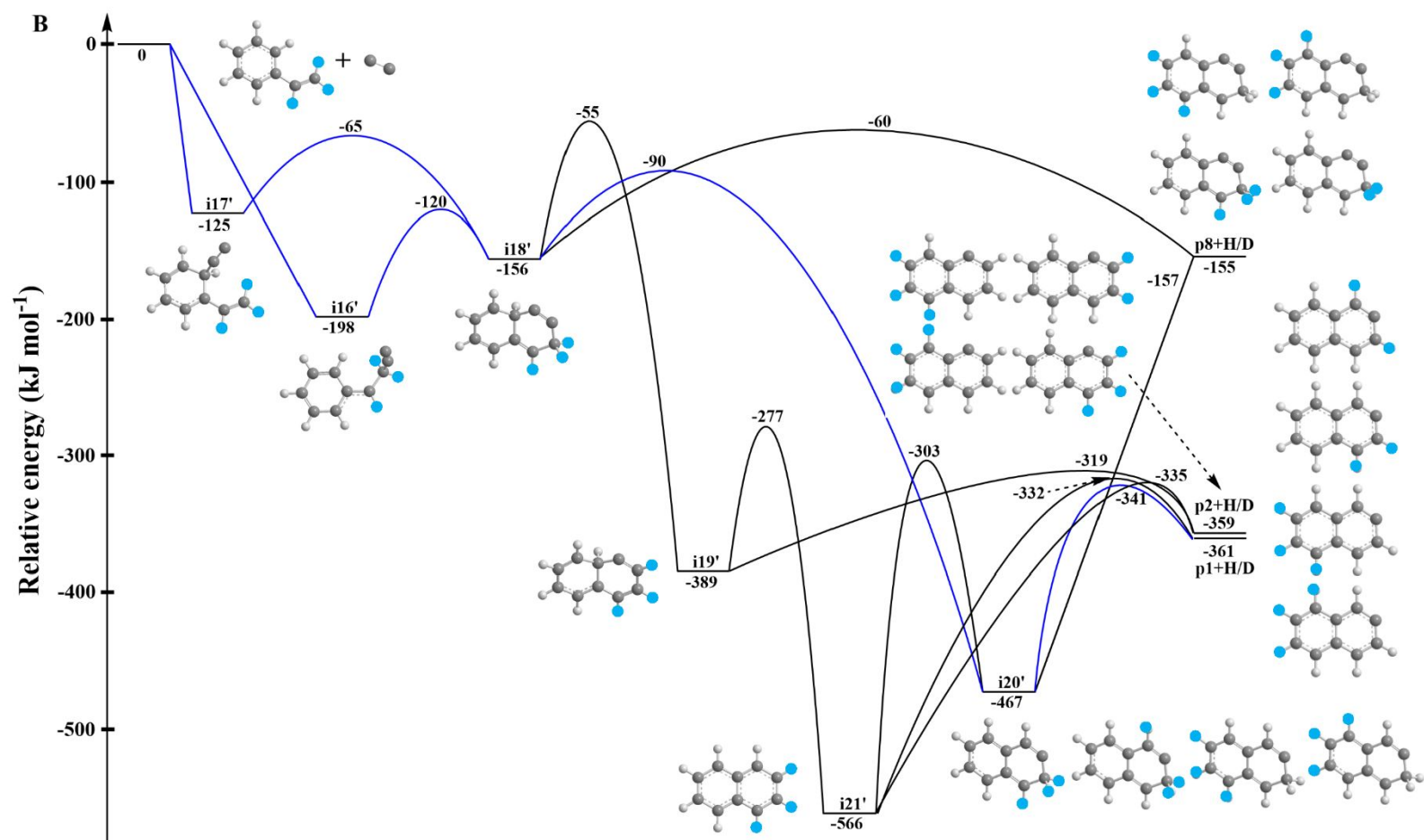


Figure S5. Singlet (A) and triplet (B) PESs of the reactions of C_2 with D3/D5-styrene. For the C_2 -D3-styrene reaction, H and D atoms are color-coded in gray and light blue, respectively. For the C_2 -D5-styrene reaction, H and D atoms are color-coded in light blue and gray, respectively.

Table S5. Cartesian coordinates and frequencies (cm⁻¹) of reactants, intermediates, transition states, and products of the reaction of the atomic carbon with indene.

Structures	Coordinates				Frequencies		
Indene	C	0.426451	-0.614328	0.000000	192.1863	211.1840	387.1324
	C	0.000000	0.721619	0.000000	392.4759	427.1947	546.9275
	C	-0.497729	-1.651910	0.000000	568.4093	608.6288	710.2531
	C	1.892636	-0.624480	0.000000	737.6755	750.3792	789.2875
	C	2.349877	0.633897	0.000000	850.7764	877.5039	878.9044
	C	1.209641	1.618035	0.000000	943.0929	966.7911	967.1116
	C	-1.852851	-1.337464	0.000000	981.7757	1006.3508	1052.8206
	C	-2.275575	-0.010329	0.000000	1091.5391	1139.1635	1162.2058
	C	-1.348782	1.030281	0.000000	1185.0048	1193.9034	1239.5416
	H	-0.171648	-2.686483	0.000000	1261.7273	1323.4035	1348.4972
	H	2.497524	-1.522436	0.000000	1396.5726	1434.5001	1508.4990
	H	3.390271	0.931387	0.000000	1511.6289	1638.2473	1671.8620
	H	1.236216	2.271438	0.879805	1691.0352	3048.1553	3083.2738
	H	1.236216	2.271438	-0.879805	3184.0384	3190.8143	3202.2079
	H	-2.589597	-2.132979	0.000000	3211.2781	3217.8654	3236.4371
H	-3.336453	0.213485	0.000000				
H	-1.684544	2.062232	0.000000				
i1	C	0.031716	-0.652762	-0.106298	132.6505	179.1404	307.4657
	C	-0.039587	0.741242	-0.028277	367.7040	411.5607	455.6162
	C	-1.122793	-1.422880	-0.097372	523.8681	564.6720	607.8669
	C	1.439830	-1.128429	-0.187964	649.1044	698.6416	740.3058
	C	2.316027	0.250181	-0.193072	780.3333	803.4354	844.7559
	C	1.317348	1.405864	-0.131515	885.9966	904.7759	942.2465
	C	-2.357362	-0.790236	0.006839	967.4225	969.9985	1013.6741
	C	-2.430887	0.595437	0.100844	1029.4605	1047.6636	1061.5687
	C	-1.271434	1.366642	0.082547	1128.7796	1180.1284	1183.8905
	H	-1.061860	-2.503751	-0.162635	1190.4030	1203.1662	1233.6210
	H	1.693144	-1.931246	-0.878692	1263.1362	1270.3214	1334.5866
	H	3.134043	0.316131	-0.908639	1348.2105	1400.4946	1474.7087
	H	1.519429	2.050583	0.728558	1507.2087	1524.8831	1658.1424
	H	1.376854	2.025166	-1.031783	1680.6033	3058.7116	3102.5277
	H	-3.266829	-1.380211	0.017637	3131.2856	3138.5978	3185.0009
	H	-3.397477	1.079345	0.183050	3191.8550	3203.1686	3215.0679
	H	-1.335045	2.448142	0.143738			
	C	2.340096	-0.715752	0.872396			
i2	C	0.039521	0.753421	0.000033	88.9551	170.8604	258.1947
	C	-0.050381	-0.657342	0.000021	365.5863	425.3892	452.1345
	C	1.308966	1.356824	0.000021	479.1439	507.8105	540.9938
	C	-1.165428	1.549629	0.000011	610.7651	664.0126	723.1994
	C	-2.584034	-0.448856	-0.000079	751.6426	759.1445	780.9279
	C	-1.387401	-1.367531	0.000110	785.0626	872.2799	912.6177
	C	2.460076	0.592636	-0.000014	928.9301	969.3165	970.7058
	C	2.368927	-0.797777	-0.000046	1002.9011	1071.6552	1091.6960
	C	1.121439	-1.406541	-0.000028	1144.5909	1182.4582	1209.3261
	C	-2.372871	0.876655	-0.000070	1209.4510	1211.8659	1268.0448
	H	1.374001	2.440042	0.000035	1282.5004	1315.8028	1348.6230
	H	-1.097702	2.631247	0.000005	1378.7430	1440.7871	1478.2094
	H	-3.574685	-0.889966	-0.000165	1514.8036	1540.7294	1631.2300
	H	-1.443454	-2.034275	0.872627	1665.3465	3000.3134	3021.7262
	H	-1.443406	-2.034666	-0.872101	3178.6877	3190.4623	3199.8984
	H	3.430820	1.075120	-0.000024	3200.5976	3206.0981	3219.2778
	H	3.267712	-1.403615	-0.000085			

	H	1.053826	-2.490585	-0.000050			
i3	C	0.051694	0.748351	-0.000002	123.8292	183.1244	255.7026
	C	-0.041204	-0.684460	-0.000034	364.1223	384.1793	447.9525
	C	1.301919	1.360146	0.000021	490.4965	507.1204	535.5168
	C	-1.189325	1.521468	-0.000037	612.8209	674.7708	723.4629
	C	-2.592490	-0.575586	0.000151	755.9448	761.4884	768.7761
	C	-1.283324	-1.320770	-0.000031	829.3031	869.4038	907.9376
	C	2.467480	0.606728	-0.000003	915.4957	942.3400	953.2810
	C	2.394066	-0.793995	-0.000052	991.4524	1020.1022	1057.5157
	C	1.173337	-1.426379	-0.000073	1143.4959	1161.7703	1180.9553
	C	-2.343564	0.877376	-0.000007	1201.4456	1224.2943	1253.8176
	H	1.357907	2.444136	0.000041	1300.0446	1342.0151	1347.1108
	H	-1.127904	2.606260	-0.000031	1422.1117	1449.4791	1462.0694
	H	-3.196421	-0.866092	-0.873055	1509.2434	1584.5041	1628.8540
	H	-3.196026	-0.865897	0.873709	1694.1577	2984.1270	2999.0179
	H	-1.326281	-2.405463	-0.000090	3174.3832	3185.0770	3187.9116
	H	3.432189	1.100283	0.000016	3190.4861	3203.7146	3221.2925
	H	3.306047	-1.380372	-0.000074			
	H	1.118954	-2.510134	-0.000110			
i4	C	0.000028	-0.724621	0.000020	162.4166	165.4587	284.8216
	C	0.000035	0.724615	-0.000014	364.0562	380.4676	477.2729
	C	-1.229911	-1.396841	0.000034	482.4856	509.9762	522.9954
	C	1.229931	-1.396826	0.000063	591.6620	697.1353	698.4544
	C	2.477429	0.676528	-0.000027	704.2988	718.1336	736.5160
	C	1.229913	1.396829	-0.000041	757.8832	810.6642	813.0150
	C	-2.477459	-0.676509	0.000016	815.2723	833.7180	908.8631
	C	-2.477458	0.676504	-0.000029	946.1217	978.6458	979.3166
	C	-1.229924	1.396838	-0.000043	1061.6537	1063.9361	1111.2294
	C	2.477422	-0.676517	0.000022	1196.3572	1201.3796	1205.6005
	H	-1.238774	-2.481290	0.000076	1295.6904	1354.8151	1421.5145
	H	1.238802	-2.481276	0.000117	1429.7454	1434.7004	1470.2790
	H	3.408342	-1.231162	0.000020	1470.7648	1485.2335	1577.4581
	H	3.408347	1.231173	-0.000076	1685.2220	3192.9918	3195.6864
	H	1.238758	2.481279	-0.000048	3195.9423	3202.4011	3207.6845
	H	-3.408356	-1.231189	0.000030	3208.9481	3222.8053	3224.8040
	H	-3.408356	1.231182	-0.000045			
	H	-1.238795	2.481287	-0.000079			
i5	C	0.136574	-0.553170	-0.155374	123.2785	140.2888	193.8248
	C	0.030916	0.829762	0.041038	266.5758	336.0568	368.7548
	C	-0.986932	-1.366378	-0.236739	428.9746	473.6658	495.4364
	C	1.635039	-0.943154	-0.255883	544.3875	597.0677	701.6465
	C	2.305865	0.386383	-0.360974	727.5842	768.9376	803.3736
	C	1.386857	1.491306	0.054246	838.8232	893.5284	905.9333
	C	-2.241811	-0.775320	-0.130262	927.2588	982.7259	1008.9974
	C	-2.352226	0.597503	0.059010	1026.3560	1039.0179	1059.6835
	C	-1.220348	1.409158	0.140439	1080.1128	1120.0630	1151.4330
	C	1.371846	-1.538437	1.058738	1168.4015	1189.7889	1215.6213
	H	-0.879185	-2.435574	-0.369078	1230.0586	1280.3997	1330.8536
	H	1.865515	-1.656546	-1.057760	1337.5264	1370.8440	1448.8750
	H	3.366754	0.500023	-0.532158	1498.3165	1516.6397	1656.7519
	H	1.619961	1.866893	1.063325	1674.2745	2989.0227	3026.2976
	H	1.427557	2.358360	-0.615446	3053.5673	3191.1943	3204.6155
	H	-3.134365	-1.386485	-0.189615	3214.5117	3228.8662	3245.1102
	H	-3.335536	1.047329	0.140358			
	H	-1.325370	2.480078	0.274934			
i6	C	0.197696	-0.512745	-0.555151	170.8317	219.9144	250.0439

	C	0.216460	0.888818	-0.225637	353.8086	384.5960	394.6959
	C	-0.950155	-1.321559	-0.206862	476.9121	508.9895	548.7236
	C	1.442161	-1.132787	-0.109726	577.4427	610.4290	645.2384
	C	2.367424	-0.020826	0.127520	713.7835	741.5404	776.8171
	C	1.658444	1.299423	-0.027765	827.4128	864.8142	892.6583
	C	-2.190578	-0.562984	-0.017738	921.1968	937.2315	982.8220
	C	-2.169910	0.784547	0.092931	1005.5656	1012.7187	1044.9929
	C	-0.941814	1.537249	0.054955	1062.0344	1090.4171	1136.5833
	C	0.231170	-1.306705	0.918276	1167.1750	1202.4604	1211.6518
	H	-1.043087	-2.326464	-0.613253	1240.9537	1304.5417	1333.4198
	H	1.808137	-2.078284	-0.503669	1361.5180	1409.8941	1426.1283
	H	3.430391	-0.127177	0.285339	1449.9785	1463.8111	1595.3633
	H	1.771066	1.963501	0.836212	1688.7708	2996.6463	3066.7973
	H	2.045189	1.849933	-0.899005	3137.0725	3139.6950	3192.4088
	H	-3.127651	-1.104339	0.023654	3205.1587	3223.6351	3253.4497
	H	-3.100552	1.318814	0.250465			
	H	-0.948880	2.589427	0.315439			
i11	C	-0.468987	0.778998	0.017594	127.9246	170.8164	248.251
	C	-0.346956	-0.611194	-0.176746	312.4365	363.3863	401.067
	C	0.668883	1.625943	-0.042161	427.9579	488.4505	517.912
	C	-1.871561	1.093831	0.179959	544.8808	603.1340	683.401
	C	-2.606041	-0.032292	0.084238	722.1217	738.0388	801.042
	C	-1.718131	-1.221484	-0.154404	833.9774	840.7502	865.297
	C	1.896538	1.069721	-0.222484	934.9567	943.2621	968.499
	C	2.103250	-0.382864	-0.226587	971.3088	980.0391	993.967
	C	0.882403	-1.227762	-0.345699	1080.6092	1105.0337	1152.478
	H	0.550413	2.701073	0.027535	1160.4480	1177.6505	1235.361
	H	-2.258367	2.090696	0.347370	1255.4079	1309.1454	1332.935
	H	-3.682643	-0.098553	0.162567	1381.4659	1431.4198	1446.745
	H	-1.798070	-1.964898	0.646510	1502.2353	1528.3743	1580.003
	H	-1.956214	-1.736228	-1.092377	1632.0642	3057.5520	3094.761
	H	2.775705	1.700993	-0.292893	3107.7772	3194.4368	3214.160
	H	2.986342	-0.748517	-0.751661	3219.1763	3224.2054	3247.057
	H	0.961505	-2.265440	-0.642697			
	C	1.864156	-1.039418	1.152232			
i9	C	-0.443663	0.733989	-0.054889	133.8902	166.6935	229.6354
	C	-0.451205	-0.699765	-0.104866	314.8853	366.5473	382.5681
	C	0.733567	1.452758	-0.216753	404.7490	459.3190	505.7798
	C	-1.811452	1.186710	0.097278	547.8877	589.0043	685.0594
	C	-2.638606	0.126841	0.135490	735.0830	745.0746	813.2560
	C	-1.880226	-1.167520	0.012053	825.0631	851.5513	870.0438
	C	1.949107	0.778823	-0.329844	946.4850	952.7198	957.9795
	C	1.989393	-0.701698	-0.218889	963.7182	967.0533	986.4574
	C	0.697788	-1.397645	-0.257982	1062.8538	1107.1943	1161.3078
	H	0.709545	2.535377	-0.282715	1162.7177	1170.6323	1237.7200
	H	-2.106485	2.225534	0.168877	1259.7121	1311.4829	1340.7647
	H	-3.714477	0.173524	0.242572	1386.0080	1414.5805	1441.7774
	H	-2.029631	-1.807394	0.888993	1481.6767	1549.0606	1616.7379
	H	-2.202082	-1.745204	-0.861996	1658.1043	3049.5168	3085.4454
	H	2.851589	1.316178	-0.587857	3094.2665	3196.3069	3198.3881
	H	2.824555	-1.188728	-0.724599	3222.3017	3227.1272	3244.2518
	H	0.697338	-2.480372	-0.331323			
	C	2.350239	-0.150645	1.186410			
i7	C	0.256393	-0.598323	-0.160196	154.2705	175.1092	210.1544
	C	0.325359	0.799588	0.058845	321.5049	353.8020	375.6961
	C	-1.050166	-1.273218	-0.221003	415.7079	485.9464	535.5648

	C	1.605296	-1.112488	-0.316110	577.8291	618.6546	654.2818
	C	2.484618	-0.106850	-0.163204	721.2720	740.0365	767.7976
	C	1.776868	1.192694	0.114486	833.8149	864.8693	889.8476
	C	-2.199613	-0.363852	-0.330127	936.9728	954.0235	966.6753
	C	-2.081377	0.970224	-0.107677	973.9143	995.6783	1027.4444
	C	-0.806237	1.574366	0.114167	1062.9133	1106.0490	1154.2138
	C	-0.559677	-1.490114	1.241298	1164.6805	1197.0645	1215.0330
	H	-1.098705	-2.204110	-0.789318	1239.3123	1304.7211	1336.3236
	H	1.837284	-2.152387	-0.498686	1412.0729	1426.0297	1442.2578
	H	3.561413	-0.197213	-0.209957	1459.1009	1552.2095	1605.3100
	H	2.043806	1.592632	1.100355	1645.5436	3050.7710	3087.2976
	H	2.020547	1.968733	-0.619462	3093.0306	3190.6267	3205.4595
	H	-3.172221	-0.802820	-0.521216	3216.0344	3230.4104	3253.4745
	H	-2.963835	1.599241	-0.123858			
	H	-0.737071	2.643761	0.279261			
i12	C	-0.396885	-0.709484	0.000028	114.1477	160.9781	244.6709
	C	-0.520541	0.722647	0.000000	332.8722	383.8029	397.4290
	C	0.784492	-1.501974	-0.000035	428.2240	482.9080	540.5834
	C	-1.730925	-1.260737	0.000003	609.7097	634.8185	663.6078
	C	-2.665537	-0.289461	0.000061	675.3084	747.8504	767.1480
	C	-1.999212	1.056307	0.000033	788.5533	847.1270	857.5543
	C	2.093407	-1.120507	-0.000059	935.7370	935.9903	947.9448
	C	2.605234	0.242500	-0.000004	960.9928	984.2109	985.3708
	C	0.464509	1.669542	-0.000048	1070.1646	1085.1144	1138.9287
	C	1.844798	1.332993	0.000023	1165.0748	1207.1100	1248.6202
	H	0.605306	-2.575113	-0.000082	1283.0913	1310.3813	1367.2274
	H	-1.931821	-2.325655	-0.000005	1400.5240	1437.6971	1449.5138
	H	-3.737299	-0.430556	0.000104	1513.6203	1567.7537	1634.2570
	H	-2.263887	1.655161	-0.879363	1683.6053	3039.8112	3073.4709
	H	-2.263790	1.655046	0.879543	3154.0329	3162.1212	3172.3052
	H	2.841005	-1.906842	-0.000122	3200.3670	3212.5184	3246.4955
	H	3.686877	0.357670	0.000010			
	H	0.187575	2.719333	-0.000104			
i10	C	0.420195	0.725909	-0.000076	116.4697	168.0360	241.9397
	C	0.442338	-0.699133	0.000144	329.2430	350.5724	392.4011
	C	-0.710981	1.606724	-0.000227	422.1534	490.3283	550.3685
	C	1.787006	1.194775	0.000237	592.0014	643.1158	667.8794
	C	2.656553	0.165348	-0.000101	681.8162	748.1787	760.2453
	C	1.896727	-1.127819	0.000189	786.4012	837.5092	888.3812
	C	-2.028030	1.281098	-0.000278	926.8271	931.1446	938.0179
	C	-1.997425	-1.294012	0.000024	947.8769	984.8627	990.8629
	C	-0.587249	-1.611201	0.000223	1069.4738	1112.0270	1137.4524
	C	-2.509964	-0.064630	-0.000196	1160.5813	1209.1610	1232.4346
	H	-0.471726	2.668202	-0.000204	1271.0047	1324.2373	1346.3140
	H	2.053153	2.245370	0.000277	1390.0596	1430.5324	1444.5548
	H	3.735240	0.233976	-0.000204	1502.7625	1564.6814	1635.3846
	H	2.121330	-1.743198	-0.879124	1684.2449	3042.1617	3076.4963
	H	2.121470	-1.743195	0.879462	3146.6188	3156.2441	3178.8801
	H	-2.761927	2.080175	-0.000311	3196.1786	3206.3924	3247.2844
	H	-2.684758	-2.138305	0.000064			
	H	-0.327809	-2.665384	0.000404			
i8	C	-0.517466	-0.764695	-0.000002	130.6767	156.5773	240.8473
	C	-0.503790	0.652721	0.000069	321.6115	381.9106	390.7362
	C	1.971332	-1.333577	-0.000017	426.4620	495.3923	571.9389
	C	-1.887810	-1.220773	-0.000130	574.5524	639.0048	666.9901
	C	-2.732763	-0.169793	0.000132	677.3253	714.1910	745.4681

	C	-1.947629	1.110024	-0.000113	798.3778	866.7706	877.4069
	C	2.591295	-0.012383	-0.000048	926.5042	927.5917	943.5733
	C	1.967076	1.194208	0.000026	950.1882	981.1423	1005.9647
	C	0.570629	1.520006	0.000123	1052.7396	1101.0671	1132.8688
	C	0.658079	-1.546007	0.000029	1154.7301	1220.4963	1235.3474
	H	2.644689	-2.187286	-0.000019	1276.5670	1301.8863	1370.9908
	H	-2.168151	-2.266027	-0.000213	1381.3815	1427.0683	1449.1877
	H	-3.812668	-0.215145	0.000188	1508.5872	1571.2759	1630.2953
	H	-2.159060	1.729270	-0.879860	1673.4816	3045.4080	3081.1514
	H	-2.159110	1.729474	0.879468	3156.3359	3161.8649	3180.4655
	H	3.676789	-0.007416	-0.000142	3196.6036	3222.9564	3250.9771
	H	2.626485	2.058388	-0.000010			
	H	0.337311	2.580355	0.000166			
ts_i1_i2	C	0.006042	-0.717489	0.064590	-869.3945	137.1567	168.0067
	C	-0.001172	0.688020	-0.010875	288.4855	362.7807	419.4518
	C	1.228733	-1.396159	0.112389	459.9178	504.8266	539.1919
	C	-1.301105	-1.343450	0.096290	611.3828	617.0385	656.7874
	C	-2.467271	0.346391	0.125846	730.9054	765.3053	780.9858
	C	-1.339851	1.352292	0.197736	830.3782	873.7582	908.1145
	C	2.416817	-0.688861	0.021566	947.0529	966.8615	981.2842
	C	2.403656	0.698792	-0.106827	1005.1919	1060.8329	1096.2423
	C	1.195278	1.384637	-0.112510	1136.2295	1173.3222	1178.2822
	C	-2.364020	-0.729880	-0.715475	1187.6799	1196.3954	1222.3914
	H	1.239240	-2.477961	0.187784	1265.3552	1290.7871	1341.3374
	H	-1.529713	-2.143736	0.794429	1345.8619	1446.0539	1469.5140
	H	-3.370697	0.580305	0.700544	1502.9307	1513.6654	1632.4911
	H	-1.531930	2.114559	-0.567161	1665.2012	3042.5890	3060.2636
	H	-1.355076	1.867818	1.164558	3083.2014	3174.8055	3184.9511
	H	3.361902	-1.219916	0.039537	3194.1753	3206.7722	3220.1761
	H	3.336810	1.244529	-0.184897			
	H	1.186819	2.468645	-0.171175			
ts_i2_p1	C	0.020857	0.762005	0.014592	-903.3951	169.3056	182.7541
	C	-0.072471	-0.653435	-0.034576	279.0263	364.6448	391.3104
	C	1.301035	1.366098	0.039657	426.5813	481.6588	509.7036
	C	-1.180340	1.537216	0.021059	516.7515	525.6829	616.2027
	C	-2.515986	-0.506604	-0.106822	632.4179	752.6574	776.8362
	C	-1.362004	-1.277909	-0.033774	785.2030	798.9530	829.7284
	C	2.435119	0.599193	0.010576	853.9905	895.6756	939.6080
	C	2.342754	-0.807441	-0.043218	980.0114	1011.8699	1015.7064
	C	1.116559	-1.417317	-0.062350	1050.8478	1062.3577	1142.4018
	C	-2.353534	0.870295	-0.048726	1163.6707	1174.9343	1213.8299
	H	1.369497	2.448040	0.080806	1246.6777	1285.4896	1340.3394
	H	-1.121957	2.619932	0.063522	1387.1293	1412.5556	1467.4137
	H	-3.492317	-0.971272	-0.173194	1478.2452	1542.7945	1606.8153
	H	-1.426305	-1.749291	1.816522	1644.8541	1694.9681	3187.3931
	H	-1.420338	-2.349467	-0.195194	3189.5975	3190.8624	3193.6703
	H	3.410164	1.072529	0.028924	3205.7146	3213.1826	3220.4324
	H	3.247585	-1.403747	-0.066142			
	H	1.041740	-2.499325	-0.093742			
ts_i2_i3	C	0.040726	0.739225	0.007738	-2083.5008	155.9346	175.8806
	C	-0.032858	-0.681530	0.000402	333.3027	368.4893	451.5275
	C	1.285619	1.358040	0.017015	465.0583	486.3272	514.4181
	C	-1.207497	1.521488	-0.004416	558.6216	607.8537	630.8254
	C	-2.584768	-0.521401	-0.023531	726.9919	755.7372	761.7807
	C	-1.315893	-1.344703	0.014182	773.6746	798.1974	831.9535
	C	2.460174	0.610653	0.005626	876.7781	913.5413	947.0062

	C	2.392327	-0.776327	-0.019943	970.3910	994.1724	1069.3194
	C	1.159911	-1.414737	-0.023792	1075.8375	1144.6632	1182.8569
	C	-2.369031	0.868419	-0.065172	1192.1373	1208.4321	1225.1772
	H	1.333681	2.442162	0.025700	1255.6910	1292.2838	1333.2749
	H	-1.144022	2.603980	0.027470	1360.0730	1392.0773	1487.7107
	H	-3.510922	-1.003112	-0.305594	1512.3725	1587.1673	1629.6138
	H	-2.090612	-1.038281	1.038821	1649.0377	2188.9007	3185.1790
	H	-1.395155	-2.407633	-0.174249	3190.2238	3191.9882	3202.8424
	H	3.421035	1.111727	0.012117	3217.5344	3221.1236	3231.0408
	H	3.302679	-1.364955	-0.033113			
	H	1.111057	-2.498643	-0.039801			
ts_i3_i4	C	-0.027801	0.737958	-0.018792	-1891.2595	160.0934	174.7066
	C	0.037117	-0.692512	-0.032336	332.0694	372.6720	464.5843
	C	-1.280102	1.363004	0.020034	493.0669	512.3794	514.5539
	C	1.197902	1.507819	-0.095289	591.7468	614.8957	625.1397
	C	2.494112	-0.617303	-0.000534	666.8472	761.0849	767.0784
	C	1.305542	-1.363649	-0.065221	771.4357	788.4000	859.7164
	C	-2.450775	0.622095	0.036439	871.8810	924.1659	948.2539
	C	-2.392661	-0.770546	0.018142	992.6037	1004.1409	1069.9190
	C	-1.167574	-1.413566	-0.014431	1087.4545	1120.5850	1151.1631
	C	2.371418	0.803655	-0.014218	1187.0699	1207.1132	1228.8475
	H	-1.322872	2.447109	0.034167	1270.1466	1300.9128	1335.0171
	H	1.167897	2.586262	-0.177440	1419.4652	1427.6952	1465.7363
	H	2.651123	0.150517	1.147211	1498.1706	1526.5561	1606.1387
	H	3.473379	-1.078491	-0.058770	1638.0283	1661.8216	3185.5557
	H	1.349046	-2.444444	-0.018922	3191.9957	3203.3609	3205.5746
	H	-3.409496	1.126953	0.066044	3218.9551	3219.0571	3221.9111
	H	-3.307619	-1.351850	0.031781			
	H	-1.124524	-2.497782	-0.026831			
ts_i4_p2	C	-0.029892	-0.732596	-0.022298	-1031.7736	168.4649	179.5236
	C	0.002417	0.690960	0.028532	310.9748	359.2952	401.2921
	C	-1.269170	-1.405961	-0.068071	426.5259	475.8863	510.6120
	C	1.231517	-1.372812	0.018638	518.4151	537.3023	620.2435
	C	2.439847	0.664280	-0.067204	637.8059	738.0893	777.8502
	C	1.259476	1.356297	0.030546	788.0924	796.4199	805.4181
	C	-2.439611	-0.692773	-0.066574	875.5480	904.1855	933.1487
	C	-2.418319	0.716417	-0.001958	981.8292	992.3992	1015.8128
	C	-1.227605	1.391463	0.047990	1046.5154	1065.1460	1139.7563
	C	2.436567	-0.747836	-0.147650	1171.0869	1186.4227	1197.6147
	H	-1.276247	-2.488937	-0.101209	1241.5449	1276.4052	1370.5696
	H	1.307198	-1.579663	1.900803	1376.1099	1393.5497	1461.1413
	H	3.383575	1.196709	-0.108890	1488.4121	1531.5410	1606.2064
	H	1.269402	2.440361	0.069722	1643.5760	1692.3827	3190.3361
	H	-3.390208	-1.211852	-0.107323	3192.7108	3202.6509	3205.5772
	H	-3.353443	1.264491	0.010375	3214.4735	3217.4160	3225.6056
	H	-1.211183	2.475060	0.103451			
	H	3.359536	-1.300805	-0.278639			
ts_i4_p1	C	-0.038226	-0.692604	-0.009564	-1088.2338	165.7780	178.0286
	C	0.013484	0.730361	-0.039981	350.1976	365.8830	394.9015
	C	-1.299988	-1.357110	-0.068791	423.9728	484.9215	503.8341
	C	1.175459	-1.416041	0.037312	512.2979	534.8143	619.6877
	C	2.431987	0.642612	0.012873	633.9259	743.8968	757.9149
	C	1.275311	1.374160	-0.033954	778.7089	798.4996	809.0466
	C	-2.469431	-0.653490	-0.093501	852.1422	891.8275	937.7696
	C	-2.368358	0.751793	0.011779	973.4257	985.7544	1012.2867
	C	-1.205642	1.459967	-0.118028	1028.0497	1054.3668	1154.0310

	C	2.382348	-0.766509	0.051849	1162.6364	1177.6076	1213.5006
	H	-1.316273	-2.442208	-0.099226	1248.2944	1284.8976	1347.9583
	H	1.136676	-2.500132	0.062144	1387.6727	1414.7947	1454.0947
	H	3.392082	1.145747	0.023277	1476.4934	1546.0249	1604.8267
	H	1.309959	2.458107	-0.061404	1632.3452	1688.0140	3189.0775
	H	-3.432103	-1.149056	-0.130116	3190.5805	3194.2964	3196.3970
	H	-2.586475	0.842981	1.836656	3208.6535	3218.0901	3222.0770
	H	-1.190515	2.539719	-0.222104			
	H	3.304979	-1.333999	0.090801			
ts_i5_i6	C	0.175365	-0.513086	-0.454951	-276.5447	170.9101	213.2364
	C	0.168204	0.882832	-0.167174	279.1557	333.9276	385.2686
	C	-0.974263	-1.305549	-0.291397	408.6967	492.7684	550.7693
	C	1.491213	-1.092150	-0.143524	574.8411	594.9379	707.8760
	C	2.381025	0.073073	-0.000535	712.3764	737.2341	778.5559
	C	1.595447	1.356665	-0.012265	824.3172	878.5123	890.3442
	C	-2.202457	-0.617288	-0.049219	918.1671	935.6370	945.7690
	C	-2.211657	0.740475	0.106087	1008.2462	1016.5697	1034.4184
	C	-1.017236	1.513964	0.067163	1069.3350	1095.3627	1148.3892
	C	0.493274	-1.419832	1.024057	1178.2669	1198.4169	1211.5590
	H	-0.984521	-2.348219	-0.580361	1242.6973	1311.4079	1320.0915
	H	1.860422	-1.978986	-0.658596	1348.7672	1436.1486	1449.3301
	H	3.452391	0.012956	0.119276	1471.6752	1474.7049	1624.6149
	H	1.712829	1.940821	0.909398	1680.9791	3006.2854	3043.3072
	H	1.901009	2.016624	-0.837042	3120.7673	3193.5971	3207.8260
	H	-3.125599	-1.180467	0.006321	3215.1442	3227.9643	3253.5828
	H	-3.152959	1.246357	0.291402			
	H	-1.057057	2.576291	0.280140			
ts_i3_p1	C	0.038794	0.749882	-0.015674	-843.4879	158.7872	185.4441
	C	-0.051493	-0.671824	-0.040307	309.7309	354.1054	381.6755
	C	1.314912	1.357742	0.030925	416.7869	473.4217	506.1111
	C	-1.166453	1.520875	-0.050735	521.9768	524.8983	625.8521
	C	-2.490896	-0.545571	-0.045011	637.2300	748.9250	762.0445
	C	-1.320557	-1.295363	-0.088287	777.1382	797.3084	835.5421
	C	2.452818	0.594812	0.048705	854.0041	893.1912	939.0516
	C	2.368404	-0.814206	0.018030	979.8948	1003.1769	1012.2640
	C	1.147690	-1.430456	-0.026691	1036.4114	1054.0549	1140.1695
	C	-2.333806	0.851716	-0.082517	1165.3866	1172.6071	1213.8649
	H	1.379283	2.440548	0.052135	1249.9650	1285.9372	1336.0069
	H	-1.111072	2.604752	-0.056910	1393.9148	1416.8157	1460.3540
	H	-3.453935	-1.011886	-0.215005	1479.3018	1541.0699	1603.8154
	H	-2.974539	-0.714987	1.789115	1648.1453	1688.0256	3187.5636
	H	-1.377046	-2.378279	-0.128082	3189.8594	3190.3832	3194.1211
	H	3.425024	1.072846	0.085646	3205.7915	3207.0844	3219.5888
	H	3.276711	-1.405539	0.031150			
	H	1.079089	-2.513102	-0.048683			
ts_i1_i5	C	0.128633	-0.531269	-0.182495	-622.7608	111.5656	142.0308
	C	-0.047871	0.838813	0.017156	201.2499	350.7446	371.7059
	C	-0.950486	-1.401006	-0.226444	415.8315	445.6776	528.9851
	C	1.611833	-0.862852	-0.290141	540.3127	609.5793	705.4624
	C	2.249211	0.492368	-0.342482	738.6811	777.7184	820.4968
	C	1.276064	1.564981	0.032460	846.3457	897.8215	922.4666
	C	-2.232288	-0.876386	-0.082412	929.1462	983.4085	1018.6852
	C	-2.415846	0.488481	0.107278	1025.5870	1047.5198	1060.9450
	C	-1.325003	1.354736	0.156879	1114.0098	1120.4553	1153.6571
	C	1.841905	-1.540576	1.008370	1170.9687	1186.1143	1193.4458
	H	-0.799805	-2.463845	-0.376574	1237.3415	1270.5416	1332.1601

	H	1.867078	-1.495232	-1.155727	1338.0517	1363.1598	1454.5546
	H	3.317208	0.636957	-0.428962	1502.4930	1524.4808	1659.0752
	H	1.487689	1.973826	1.032950	1681.3810	2971.6000	2988.7513
	H	1.299732	2.417396	-0.657954	3045.1467	3189.7964	3199.8131
	H	-3.090979	-1.536689	-0.118708	3209.2572	3219.7468	3240.9667
	H	-3.419090	0.885030	0.215288			
	H	-1.478741	2.418817	0.300666			
ts_i6_i7	C	0.218991	-0.534336	-0.444691	-366.6895	183.1276	222.6003
	C	0.241709	0.872189	-0.155242	269.3138	374.5540	385.2837
	C	-0.975794	-1.313134	-0.202862	446.2472	501.5604	540.2660
	C	1.514939	-1.092335	-0.228925	597.1068	603.5712	636.8086
	C	2.411410	-0.039447	0.017567	710.8641	744.2118	787.0773
	C	1.683473	1.278608	0.034557	826.1276	873.9278	879.8521
	C	-2.203043	-0.517712	-0.099096	895.5669	936.7181	964.1043
	C	-2.162941	0.828177	0.031576	966.0744	997.1060	1043.0364
	C	-0.916889	1.546987	0.060073	1066.5839	1075.9731	1146.2976
	C	0.037058	-1.389847	1.059345	1166.8954	1209.1787	1225.6402
	H	-1.065998	-2.302242	-0.648769	1244.5152	1307.2015	1336.0817
	H	1.798033	-2.107005	-0.469809	1388.7015	1438.1300	1443.1009
	H	3.476302	-0.145259	0.163253	1453.5996	1476.5679	1593.0930
	H	1.816925	1.828373	0.973459	1684.6829	3022.3056	3065.6679
	H	2.034904	1.941247	-0.768527	3125.7486	3194.4120	3206.5705
	H	-3.152930	-1.038269	-0.120130	3224.4454	3238.7721	3256.1522
	H	-3.087920	1.383064	0.140288			
	H	-0.912797	2.605184	0.296424			
ts_i9_i10	C	-0.448181	0.736311	-0.039652	-499.9568	147.2798	165.4067
	C	-0.455477	-0.704395	-0.077099	267.1465	351.5288	386.2996
	C	0.721504	1.466601	-0.198850	396.6143	436.2275	540.8099
	C	-1.817556	1.187043	0.073117	571.1184	645.7238	687.6945
	C	-2.645383	0.126374	0.119711	735.4521	765.0421	794.8656
	C	-1.886652	-1.170111	0.035836	831.3027	844.8844	869.0863
	C	1.957676	0.818152	-0.231077	940.8995	949.6418	956.0884
	C	1.998923	-0.725545	-0.224180	965.7185	983.7698	990.5896
	C	0.682142	-1.403023	-0.259984	1055.2918	1104.5243	1149.5833
	C	2.415332	-0.186433	1.085519	1164.9813	1165.9707	1227.2653
	H	0.676097	2.543051	-0.328617	1260.9815	1279.5633	1315.2649
	H	-2.115610	2.226528	0.118826	1380.6406	1386.1995	1441.0661
	H	-3.722691	0.176037	0.211536	1457.7087	1512.4988	1608.7341
	H	-2.049161	-1.785518	0.927976	1668.0875	3047.6288	3048.9971
	H	-2.200773	-1.769599	-0.825998	3083.7738	3189.9565	3191.9339
	H	2.837019	1.359987	-0.554835	3212.6803	3219.7081	3241.5397
	H	2.767903	-1.136408	-0.887010			
	H	0.673253	-2.483929	-0.361916			
ts_i11_i12	C	-0.481977	0.763743	0.063222	-525.0593	154.4722	173.4608
	C	-0.356439	-0.622811	-0.116152	291.7665	308.6870	365.9069
	C	0.648870	1.633860	-0.004122	421.9789	488.4755	489.8378
	C	-1.887377	1.085013	0.171753	588.4585	666.2613	707.5035
	C	-2.622718	-0.038575	0.044545	714.7730	765.2701	788.3402
	C	-1.729617	-1.228464	-0.159793	826.3382	859.3029	864.8515
	C	1.873417	1.108044	-0.237050	937.9318	942.6000	968.8428
	C	2.131701	-0.350333	-0.258373	973.0582	981.3611	998.7784
	C	0.876568	-1.260466	-0.213823	1074.4156	1102.4104	1143.2769
	C	1.995500	-1.051442	1.029044	1154.7586	1176.5075	1233.3288
	H	0.509420	2.705584	0.076863	1249.2661	1270.9676	1302.1367
	H	-2.276224	2.084330	0.319134	1375.6298	1416.7049	1442.1093
	H	-3.702235	-0.099508	0.074497	1452.0247	1518.1162	1567.6929

	H	-1.854600	-1.978702	0.629320	1637.7462	3051.9525	3052.1419
	H	-1.928879	-1.733789	-1.112284	3088.4684	3192.8230	3193.8606
	H	2.734952	1.758357	-0.348753	3214.6750	3223.1519	3246.7315
	H	2.891916	-0.691061	-0.968463			
	H	0.938090	-2.276626	-0.585826			
ts_i12_p5	C	0.400730	-0.754357	-0.013653	-388.6973	152.6770	158.4576
	C	0.560398	0.729245	-0.057461	248.5089	269.5251	297.9558
	C	-0.768401	-1.500675	0.039674	339.8143	404.0637	429.2986
	C	1.700423	-1.290375	-0.039008	483.1900	549.0023	600.0489
	C	2.615225	-0.246152	-0.087630	686.1393	694.1781	713.5722
	C	1.940842	0.991152	-0.068791	759.1238	801.4750	823.0831
	C	-2.098517	-1.079872	0.051448	844.7630	879.0586	912.9979
	C	-2.575214	0.230626	0.008566	940.2220	949.1723	969.0365
	C	-0.464348	1.667976	-0.074989	995.7041	1002.1475	1076.9258
	C	-1.796806	1.356066	-0.047272	1091.0674	1152.4596	1226.4199
	H	-0.619026	-2.577453	0.073501	1275.7661	1298.3573	1316.5240
	H	1.933840	-2.345711	-0.018722	1369.5823	1433.2709	1462.1271
	H	3.690718	-0.360588	-0.119748	1484.7677	1539.8149	1579.1548
	H	2.203656	1.476227	1.991193	1592.6044	1665.1182	3149.5710
	H	2.388105	1.964952	-0.203303	3158.3185	3168.6533	3196.8809
	H	-2.849898	-1.861899	0.095163	3226.6267	3241.6434	3251.8847
	H	-3.654697	0.364648	0.022388			
	H	-0.178688	2.718023	-0.105773			
ts_i7_i8	C	0.269765	-0.625947	0.007036	-578.4166	171.9981	192.5017
	C	0.346122	0.792891	0.124583	249.2771	333.0962	363.0285
	C	-1.103126	-1.284506	-0.232556	431.1676	486.0653	511.5749
	C	1.606914	-1.127914	-0.272317	532.8648	603.5447	689.4549
	C	2.486972	-0.115127	-0.215548	737.0753	751.1196	813.7299
	C	1.798611	1.188802	0.087570	844.1836	881.7247	916.0455
	C	-2.219682	-0.312223	-0.349757	923.8691	957.8076	968.6423
	C	-2.067783	1.006201	-0.098320	987.1699	988.4779	1015.0441
	C	-0.770093	1.581702	0.127828	1040.0701	1099.7064	1150.1293
	C	-0.618430	-1.551130	1.127115	1156.8599	1192.9847	1198.6206
	H	-1.084969	-2.094505	-0.970792	1236.5626	1257.3347	1311.1499
	H	1.830971	-2.172446	-0.438311	1389.9118	1393.1961	1434.0268
	H	3.557876	-0.203629	-0.341631	1449.2420	1524.6130	1606.2296
	H	2.127775	1.594171	1.052971	1657.5215	3040.7573	3041.2377
	H	2.000986	1.958061	-0.665342	3081.7744	3188.6313	3198.0103
	H	-3.199742	-0.719189	-0.574710	3215.4212	3228.2723	3252.8225
	H	-2.929898	1.662557	-0.119819			
	H	-0.678615	2.658491	0.223819			
ts_i10_p4	C	0.427326	-0.778996	-0.014231	-669.9871	149.6453	175.6419
	C	0.466409	0.709002	-0.051416	278.9378	302.4242	328.2425
	C	-0.677266	-1.612716	0.037618	340.7003	401.9930	429.7130
	C	1.766889	-1.215213	-0.043832	488.3569	586.1777	597.4599
	C	2.599525	-0.109009	-0.087659	686.7697	696.0798	723.4565
	C	1.827949	1.072509	-0.054213	772.5208	802.1811	816.6136
	C	-2.029062	-1.247904	0.051999	829.1950	860.9199	888.9781
	C	-1.958794	1.315493	-0.041623	940.7838	957.6324	971.5955
	C	-0.593896	1.603651	-0.064517	985.6029	992.8976	1069.9817
	C	-2.465840	0.044357	0.011615	1086.2861	1209.8228	1212.7381
	H	-0.466015	-2.679477	0.066509	1252.3916	1293.7243	1319.9034
	H	2.077643	-2.250732	-0.029839	1368.1507	1429.2377	1429.8290
	H	3.680279	-0.138972	-0.120961	1481.0797	1525.0464	1547.6010
	H	2.076726	1.544133	1.891116	1625.5070	1684.6727	3160.5304
	H	2.197442	2.075280	-0.214257	3163.2926	3179.5361	3182.2850

	H	-2.767495	-2.043636	0.093959	3228.1531	3241.1500	3253.5440
	H	-2.654687	2.149347	-0.059653			
	H	-0.323342	2.657006	-0.089315			
ts_i8_p3	C	0.517849	-0.820198	-0.009777	-672.3430	146.9750	158.3418
	C	0.535178	0.671167	-0.052320	281.8845	303.3167	326.0491
	C	-1.984109	-1.298907	0.054218	340.3759	404.4945	440.4587
	C	1.858883	-1.248940	-0.037559	498.6171	590.2144	605.0789
	C	2.672966	-0.127766	-0.085244	684.0937	687.0684	706.2629
	C	1.891083	1.049101	-0.055417	748.4990	799.9702	838.1393
	C	-2.553460	-0.028294	0.011911	865.7003	886.7705	893.2101
	C	-1.923276	1.216001	-0.044727	937.9548	958.8279	991.7990
	C	-0.564345	1.518009	-0.067801	994.9132	1018.3387	1053.8412
	C	-0.633532	-1.540476	0.039610	1080.4216	1170.7110	1214.0447
	H	-2.658114	-2.149798	0.098014	1239.8218	1287.9844	1312.1463
	H	2.179379	-2.279895	-0.020547	1384.3171	1409.6291	1466.0482
	H	3.754110	-0.145609	-0.119056	1480.9483	1528.5156	1564.7634
	H	2.122563	1.535082	1.883115	1641.8343	1677.1341	3162.2077
	H	2.252267	2.053646	-0.223264	3166.7835	3180.7907	3197.4569
	H	-3.639979	-0.001675	0.027377	3232.6293	3247.9374	3260.1293
	H	-2.590232	2.071719	-0.066622			
	H	-0.323418	2.578348	-0.096376			
p1	C	-0.017603	0.744867	-0.000065	174.7110	191.9391	368.9068
	C	-0.086671	-0.686741	-0.000175	387.1416	471.8432	485.5325
	C	1.254921	1.371713	0.000237	511.3204	520.5914	611.1768
	C	-1.235908	1.492866	-0.000364	628.2606	744.9525	754.9233
	C	-2.524390	-0.593402	0.000310	767.3758	793.9531	805.9425
	C	-1.355353	-1.327170	0.000097	845.0879	887.9590	936.2458
	C	2.406862	0.622856	0.000267	956.7056	970.5860	996.6642
	C	2.342245	-0.789675	-0.000021	1039.9094	1049.6505	1141.2264
	C	1.125266	-1.426446	-0.000388	1161.1603	1172.2508	1208.0941
	C	-2.396147	0.795033	0.000061	1249.9930	1276.7413	1334.9347
	H	1.304086	2.455483	0.000216	1385.5716	1394.1306	1457.5025
	H	-1.202036	2.577588	-0.000727	1468.3565	1530.2587	1592.1810
	H	-3.492817	-1.080467	0.000048	1619.9673	1656.4690	3155.3312
	H	-1.394956	-2.412147	0.000721	3158.7415	3160.0078	3164.5357
	H	3.373165	1.114745	0.000279	3176.1842	3178.9532	3188.4097
	H	3.258959	-1.368331	0.000110			
	H	1.074266	-2.510282	-0.000404			
p2	C	-0.014294	-0.761883	-0.000017	168.0441	184.6911	363.0699
	C	0.035435	0.677500	0.000010	400.7015	466.6763	507.1903
	C	-1.273456	-1.416446	0.000010	512.2760	524.4624	619.3663
	C	1.226643	-1.409081	-0.000067	633.9413	732.3800	778.6348
	C	2.472983	0.604351	-0.000059	786.8410	798.7945	803.5742
	C	1.301611	1.322703	-0.000012	872.3706	903.3779	937.3431
	C	-2.435977	-0.685430	0.000060	980.4591	991.4903	1014.3854
	C	-2.394168	0.728826	0.000087	1041.2466	1058.0113	1148.5137
	C	-1.190851	1.391497	0.000064	1172.5475	1188.2692	1207.4658
	C	2.446291	-0.820206	-0.000092	1241.3544	1275.8201	1381.5534
	H	-1.296739	-2.499814	-0.000011	1390.7668	1406.4774	1465.4258
	H	3.369579	-1.389108	-0.000127	1500.0577	1542.8097	1620.9461
	H	3.429529	1.116099	-0.000073	1670.7290	1707.5307	3189.1218
	H	1.330351	2.407073	0.000012	3190.4639	3198.8112	3202.2413
	H	-3.394594	-1.191664	0.000079	3211.9321	3215.4344	3224.8483
	H	-3.321754	1.290095	0.000129			
	H	-1.161666	2.476341	0.000089			
p5	C	0.454156	-0.726267	0.000056	163.0053	169.2581	297.3677

	C	-0.702059	-1.499759	0.000077	338.5211	403.5272	427.9253
	C	-2.038267	-1.111073	0.000036	476.2786	551.9568	601.7429
	C	-2.546214	0.190561	-0.000036	679.9803	690.6540	714.6692
	C	-1.795573	1.333193	-0.000093	764.3468	784.9115	820.5800
	C	-0.472005	1.678925	-0.000111	822.2191	880.7676	921.2191
	C	1.761089	-1.226630	-0.000101	951.7948	955.3936	962.6498
	C	2.650176	-0.147906	0.000085	994.9237	1009.5376	1076.2491
	C	1.945446	1.059928	0.000112	1090.8273	1152.8719	1227.9916
	C	0.579226	0.766838	-0.000042	1274.3128	1301.2565	1318.1798
	H	-0.528227	-2.573573	0.000067	1371.1734	1431.9351	1467.4251
	H	-2.772173	-1.910928	0.000046	1492.2002	1551.9484	1589.9293
	H	-3.628842	0.297633	-0.000058	1608.1375	1680.6304	3146.1456
	H	-0.212755	2.736432	-0.000071	3150.1974	3159.8468	3188.2061
	H	2.025807	-2.274684	-0.000198	3217.5904	3238.4053	3247.3685
	H	3.729282	-0.235025	0.000123			
	H	2.371053	2.053280	0.000187			
p3	C	-0.570864	-0.791861	0.000060	141.5968	163.4055	327.2208
	C	-0.556558	0.707748	-0.000033	327.8938	403.3535	439.9262
	C	1.923716	-1.321234	0.000054	498.3696	583.0058	607.1045
	C	-1.912282	-1.186052	-0.000168	682.0846	697.3129	704.6402
	C	-2.702559	-0.031258	0.000052	728.2292	777.1773	818.5758
	C	-1.896751	1.110214	0.000128	836.6504	882.1566	891.6967
	C	2.520809	-0.059160	-0.000007	951.2938	952.8472	986.4235
	C	1.916910	1.196267	-0.000063	1000.2086	1017.3822	1054.1547
	C	0.563269	1.528230	-0.000076	1083.3542	1175.6800	1222.2435
	C	0.572345	-1.535299	0.000068	1238.1796	1303.3705	1316.7597
	H	2.581666	-2.186071	0.000062	1388.4775	1414.1124	1474.8477
	H	-2.262390	-2.207508	-0.000320	1494.4339	1535.7484	1573.4609
	H	-3.785017	-0.025045	0.000064	1649.5046	1692.9000	3159.5235
	H	-2.238473	2.136053	0.000232	3162.7052	3178.3482	3197.7421
	H	3.607815	-0.056256	-0.000010	3225.4314	3242.6968	3259.2541
	H	2.601227	2.038695	-0.000077			
	H	0.346963	2.594562	-0.000049			
p4	C	-0.482398	0.748678	-0.000031	150.2204	180.9594	321.5879
	C	-0.482406	-0.748638	0.000044	337.1782	400.4124	409.5618
	C	0.605551	1.611482	-0.000037	488.6679	591.4410	596.5345
	C	-1.825711	1.143266	0.000046	685.8514	706.8377	719.5409
	C	-2.628346	0.000011	-0.000028	755.4884	782.6297	807.5143
	C	-1.825838	-1.143198	-0.000024	814.2010	845.3040	862.7518
	C	1.962539	1.283459	-0.000001	948.3357	959.1681	969.3330
	C	1.962510	-1.283511	-0.000002	986.3859	987.6805	1072.3587
	C	0.605397	-1.611471	0.000032	1086.9622	1212.1689	1216.9744
	C	2.435087	-0.000083	0.000003	1264.1775	1310.3531	1320.0388
	H	0.367097	2.673112	-0.000033	1369.4998	1428.9435	1442.5348
	H	-2.171144	2.167878	0.000077	1489.9862	1542.4950	1551.4857
	H	-3.710703	0.000078	-0.000058	1644.5730	1685.3080	3158.5207
	H	-2.171251	-2.167815	-0.000013	3158.8363	3178.0035	3180.8288
	H	2.680454	2.098956	0.000036	3223.9211	3237.5523	3249.5970
	H	2.680334	-2.099091	-0.000043			
	H	0.366912	-2.673093	0.000018			

Table S6. Cartesian coordinates and frequencies (cm⁻¹) of reactants, intermediates, transition states, and products of the reaction of the singlet dicarbon (C₂, X¹Σ_g⁺) with styrene.

Structures	Coordinates			Frequencies			
Styrene	C	0.514046	-0.220422	-0.002888	35.3757	205.2452	235.4052
	C	-0.406082	-1.279246	0.000138	411.9531	446.3442	448.8429
	C	-1.778225	-1.044039	0.002937	561.4898	635.0096	655.4358
	C	-2.261384	0.261196	0.002283	710.5811	787.4429	798.7095
	C	-1.359664	1.326960	-0.001276	849.8200	927.6641	930.4721
	C	0.008594	1.090363	-0.003925	976.3294	998.8183	1014.9399
	C	1.953290	-0.528216	-0.004599	1030.0462	1040.1559	1056.1697
	C	2.972003	0.334803	0.006259	1111.8838	1182.6896	1205.3639
	H	-0.035896	-2.299492	0.000677	1226.7313	1318.0793	1345.5572
	H	-2.468403	-1.880365	0.005433	1362.6204	1452.0525	1483.2868
	H	-3.328938	0.449713	0.004174	1528.6315	1618.1117	1644.4888
	H	-1.727932	2.346982	-0.002467	1691.0547	3128.5909	3142.8072
	H	0.691241	1.932066	-0.007837	3157.0921	3163.5676	3173.4637
	H	2.185844	-1.590967	-0.015687	3182.0512	3190.6412	3221.9594
i1'	C	0.592713	-0.637054	-0.075052	104.4579	107.1041	152.2489
	C	-0.283474	-1.579547	0.338827	173.6933	233.1899	267.3853
	C	-1.716233	-1.399062	0.273528	372.3938	436.3144	518.7362
	C	-2.265519	-0.270766	-0.195351	545.7249	568.8260	604.8295
	C	-1.416953	0.868496	-0.606333	677.9994	721.4941	757.3906
	C	0.086468	0.651085	-0.576674	786.5338	870.6427	931.3754
	C	2.036201	-0.879998	-0.069313	935.7140	969.1521	975.5804
	C	2.973962	0.058812	-0.183917	1011.5179	1027.4058	1031.9621
	C	0.306533	2.089017	1.032193	1049.7558	1075.1287	1129.6390
	C	-0.708784	1.645842	0.417358	1168.8213	1212.1232	1234.8435
	H	0.097913	-2.526164	0.706718	1323.0302	1350.3031	1379.3127
	H	-2.352302	-2.221250	0.580576	1437.2405	1450.2119	1463.0666
	H	-3.338030	-0.163694	-0.302394	1641.2801	1700.7473	1735.8537
	H	-1.795124	1.476745	-1.423652	1953.6095	3150.9215	3157.3462
i2'	C	0.243819	-0.575831	0.000227	71.6876	92.2780	124.8944
	C	1.494065	-1.254493	0.000001	171.4812	214.9495	221.5451
	C	2.679345	-0.557543	-0.000247	356.8062	407.7068	451.9854
	C	2.664757	0.841537	-0.000188	485.4891	543.2888	628.4147
	C	1.456562	1.528227	0.000113	690.4422	713.8642	762.7866
	C	0.252739	0.842616	0.000342	778.8278	823.6000	864.4160
	C	-2.786942	0.425326	-0.000253	917.3851	960.9950	1005.9276
	C	-3.239412	1.605125	-0.000100	1011.2195	1035.1460	1038.0847
	C	-0.930688	-1.352584	0.000316	1061.0619	1102.4691	1124.3356
	C	-2.342653	-0.938044	-0.000202	1190.5907	1206.9711	1243.7855
	H	1.501809	-2.339570	-0.000047	1290.2352	1306.9837	1365.1584
	H	3.623006	-1.090102	-0.000490	1368.4335	1455.8718	1502.5623
	H	3.599814	1.389994	-0.000328	1536.0434	1615.5888	1648.4268
	H	1.449371	2.611698	0.000224	1990.4222	2952.5537	2966.5893
H	-0.682229	1.385272	0.000669	3169.1611	3186.7680	3197.1193	
H	-0.794909	-2.431285	0.000654	3209.8907	3219.3256	3236.4477	
H	-2.822886	-1.456009	-0.852728				
H	-2.823527	-1.456011	0.851987				

i3'	C	-0.047152	-0.779395	0.034238	92.6761	122.8495	143.9553
	C	1.214974	-1.394064	-0.024052	188.5224	273.0412	297.6875
	C	2.382136	-0.667765	-0.091735	393.5129	407.1388	462.0891
	C	2.378143	0.743790	-0.068783	475.2723	540.9113	592.8698
	C	1.194064	1.401798	0.027735	596.4116	671.5369	680.2196
	C	-0.097312	0.696242	0.169609	749.5871	777.8966	833.3056
	C	-1.211729	-1.634580	0.042589	848.1960	913.1978	1019.6138
	C	-2.496143	-1.255563	-0.064081	1031.3533	1040.9856	1051.0085
	C	-2.341815	2.129211	-0.142603	1053.1347	1064.7389	1129.6956
	C	-1.298529	1.457302	-0.034847	1172.9440	1203.5700	1227.5632
	H	1.258159	-2.476839	-0.062495	1263.7448	1347.8110	1386.7346
	H	3.327753	-1.194208	-0.161839	1430.3321	1467.2516	1490.8887
	H	3.309778	1.291402	-0.136770	1561.5223	1669.0882	1673.4755
	H	1.136845	2.483112	0.064283	2077.9127	2706.3270	3137.5316
	H	-0.053547	0.643304	1.309941	3156.6030	3192.5448	3206.5544
	H	-0.984239	-2.695606	0.115247	3215.8800	3230.5432	3249.6270
	H	-2.786606	-0.214540	-0.156712			
	H	-3.267969	-2.018475	-0.060076			
i4'	C	0.130952	-0.922900	0.142718	65.7552	159.4514	171.5829
	C	1.534188	-1.301352	0.102828	218.1796	338.3448	385.4051
	C	2.453313	-0.337760	-0.075259	448.4974	494.8511	516.1820
	C	2.067150	1.065055	-0.247473	560.1180	664.9378	676.2153
	C	0.818512	1.484585	-0.022660	709.3976	788.4177	840.0897
	C	-0.194886	0.511404	0.516732	850.5035	871.5448	925.7803
	C	-0.958769	-1.622739	-0.170102	964.5458	975.7815	996.4695
	C	-2.214052	-0.786075	-0.154683	1005.8883	1011.9363	1048.2761
	C	-2.294639	1.729654	-0.159344	1103.9575	1170.7771	1179.7238
	C	-1.652114	0.624976	0.060730	1195.6373	1211.3167	1246.2175
	H	1.811803	-2.348968	0.135396	1300.3061	1306.6378	1353.3507
	H	3.503473	-0.594898	-0.157232	1402.0781	1450.4050	1483.0529
	H	2.825854	1.767275	-0.574491	1646.6725	1700.7403	1744.4531
	H	0.537516	2.523606	-0.148941	1790.0256	2971.0426	3045.9743
	H	-0.174257	0.594033	1.616207	3101.8246	3185.2871	3193.2519
	H	-0.975863	-2.677995	-0.414839	3208.1036	3213.6975	3215.5778
	H	-2.783589	-0.863404	-1.083486			
	H	-2.882868	-1.068728	0.666465			
i5'	C	0.119528	0.652846	0.189469	115.9072	167.3119	254.6363
	C	-1.115935	1.442017	0.204632	316.6929	354.0662	375.6027
	C	-2.301395	0.861088	-0.037300	434.2977	486.9764	498.2244
	C	-2.400892	-0.565403	-0.343656	545.6280	639.8315	673.7203
	C	-1.361912	-1.380932	-0.154208	708.5317	773.4181	818.3836
	C	-0.103863	-0.856496	0.487482	836.7424	887.5765	951.5440
	C	1.309718	1.208616	-0.080091	972.3277	979.9778	995.3624
	C	2.641065	0.468016	-0.277521	1003.1141	1007.5253	1046.8636
	C	2.262606	-0.938836	-0.073700	1154.5362	1158.4718	1185.6328
	C	1.195928	-1.464214	0.141359	1191.4318	1211.6010	1247.2926
	H	-1.044464	2.517177	0.331845	1296.0878	1303.3784	1339.9677
	H	-3.202203	1.463543	-0.074024	1398.3806	1450.9649	1478.8467
	H	-3.333721	-0.946189	-0.744096	1654.5883	1685.0263	1732.9305
	H	-1.414293	-2.439149	-0.381614	2250.7220	2977.2597	3052.2854
	H	-0.255693	-0.935726	1.576625	3085.8181	3167.6882	3180.7416
	H	1.356017	2.288015	-0.202349	3190.2534	3204.7513	3215.5054
	H	3.033151	0.667035	-1.279812			
	H	3.392124	0.825087	0.434624			
i9'	C	0.135694	-0.603066	0.214989	45.4581	104.2161	157.6809
	C	1.263693	-1.309693	-0.219595	203.6585	252.1818	328.1628

	C	2.478356	-0.667738	-0.396427	420.7073	434.5579	487.4880
	C	2.595409	0.692662	-0.125015	521.4320	635.3202	644.9753
	C	1.493610	1.399230	0.335053	685.7419	723.6688	766.4412
	C	0.274486	0.755271	0.509510	801.5971	831.3337	869.8482
	C	-2.705993	0.500520	-0.340818	947.8442	955.7756	999.8126
	C	-2.202550	1.692889	-0.465086	1003.4868	1006.2025	1023.2520
	C	-1.140780	-1.314493	0.347491	1025.8794	1063.4552	1124.0353
	C	-2.372216	-0.843471	0.111312	1189.5198	1217.1430	1221.3455
	H	1.175785	-2.370106	-0.433151	1263.0645	1346.9344	1362.3429
	H	3.338195	-1.227631	-0.746248	1439.2070	1490.6658	1543.8173
	H	3.545717	1.195232	-0.263652	1650.6134	1680.6102	1707.2504
	H	1.578122	2.454400	0.566829	1798.6456	2994.7457	3167.9934
	H	-0.555241	1.314379	0.931883	3169.3925	3182.4023	3194.5807
	H	-3.722266	0.702388	-0.734474	3206.3166	3206.8306	3217.4959
	H	-1.066268	-2.364113	0.619134			
	H	-3.212300	-1.517206	0.231189			
i11'	C	-0.023673	0.856431	0.151479	137.1334	152.4344	262.3705
	C	-1.366301	1.385005	-0.025658	366.3263	412.0449	458.0775
	C	-2.393768	0.533612	-0.188242	525.9319	527.7058	560.9994
	C	-2.189461	-0.917547	-0.230928	652.2443	681.6300	708.5223
	C	-1.022483	-1.473445	0.107462	741.0579	790.7761	812.2807
	C	0.071834	-0.603930	0.660432	853.9797	896.1099	902.3248
	C	1.168819	1.410637	-0.120536	968.4001	968.5255	987.0128
	C	2.274685	0.414232	0.129420	1000.3685	1004.3397	1009.6076
	C	2.313459	-0.850491	-0.697978	1041.8102	1099.0812	1128.1231
	C	1.481824	-0.853765	0.297817	1173.3747	1180.2714	1208.7220
	H	-1.512138	2.457804	-0.094786	1236.5661	1286.4327	1308.0128
	H	-3.394204	0.915544	-0.359290	1333.8186	1397.7573	1447.8871
	H	-3.012339	-1.538728	-0.567902	1641.2298	1670.8608	1726.8296
	H	-0.869997	-2.546049	0.065308	1818.4350	2972.0088	3128.3643
	H	-0.052159	-0.561571	1.755976	3180.0908	3187.1451	3202.5948
	H	1.306883	2.442659	-0.422645	3203.8740	3210.8677	3260.4268
	H	2.550258	-1.260795	-1.666911			
	H	3.094093	0.686695	0.790640			
i12'	C	0.078867	-0.715847	0.282622	108.6321	162.3844	328.8199
	C	1.231282	-1.412525	0.064368	368.7938	415.5845	429.5151
	C	2.329128	-0.668267	-0.518117	471.8653	521.4917	559.4178
	C	2.371215	0.627673	-0.183368	588.9352	659.1281	685.5750
	C	1.450949	1.420126	0.323124	719.0835	740.6640	806.1624
	C	0.044585	0.794724	0.396891	849.9212	859.9737	889.1697
	C	-1.210405	-1.377358	0.297945	919.2981	994.4612	995.7045
	C	-2.329277	-0.706302	-0.044071	1009.7513	1056.9894	1067.4358
	C	-2.280255	0.696381	-0.412267	1102.6258	1153.5630	1179.1087
	C	-1.159257	1.410984	-0.241906	1182.1140	1191.5900	1227.1158
	H	1.213024	-2.498574	0.059350	1257.8746	1304.5475	1378.0888
	H	2.885944	-1.100222	-1.343717	1405.7008	1432.2728	1463.7754
	H	1.650037	2.276683	0.957962	1573.5169	1616.6634	1712.5016
	H	-0.105107	0.956922	1.483139	1825.1291	2930.6783	3169.2102
	H	-1.238861	-2.448850	0.466787	3178.7707	3180.5458	3182.4502
	H	-3.275892	-1.230838	-0.108389			
	H	-3.170127	1.160180	-0.822810			
	H	-1.120007	2.467160	-0.483649			
i7'	C	0.230945	0.903108	0.553367	177.8744	213.9970	342.3747
	C	-0.705146	1.535536	-0.169964	380.5748	460.6745	492.0535
	C	-1.994220	0.885458	-0.446141	530.3304	546.3067	579.9159
	C	-2.152776	-0.435899	-0.301954	630.8166	713.1050	726.9409

	C	-1.080517	-1.271743	0.337508	769.7901	791.1195	838.6256
	C	-0.030352	-0.454395	1.079101	865.9316	900.6778	917.9828
	C	1.443741	-1.090927	-0.793061	951.4204	973.5444	982.7455
	C	0.338548	-1.285062	-0.082737	994.0361	1009.0095	1014.9868
	C	1.700150	1.067831	0.312310	1045.5326	1068.9168	1115.2804
	C	2.291748	0.039940	-0.330279	1134.6608	1175.3789	1206.6372
	H	-0.463339	2.449865	-0.703277	1279.8984	1301.7998	1366.9492
	H	-2.805573	1.485096	-0.844168	1382.7585	1398.2809	1422.2075
	H	-3.101024	-0.909519	-0.531733	1605.6461	1662.2727	1713.8650
	H	-1.436551	-2.152706	0.862462	1782.3915	3141.6626	3164.4023
	H	0.319349	-0.734364	2.069623	3176.4678	3180.8925	3186.0801
	H	1.661815	-1.572411	-1.740497	3189.8517	3206.2341	3209.3315
	H	2.237216	1.976571	0.559451			
	H	3.335378	0.094383	-0.620762			
i6'	C	-0.041431	-0.759365	-0.085971	72.1252	132.4997	162.1645
	C	-1.326419	-1.312138	-0.083994	211.8713	260.4305	376.5652
	C	-2.464090	-0.528545	0.017485	395.4320	451.0413	515.5800
	C	-2.343678	0.852878	0.106085	541.4944	573.0253	626.2608
	C	-1.085580	1.429303	0.083534	666.2548	679.6324	712.4939
	C	0.070713	0.644783	-0.014826	727.1338	781.6477	800.7428
	C	1.093882	-1.697373	-0.174066	840.0685	907.5277	979.4672
	C	2.322531	-1.540225	0.310091	985.9840	1017.2586	1039.1294
	C	2.332661	1.985280	-0.139961	1060.4033	1081.0586	1149.8945
	C	1.323229	1.337319	-0.078635	1193.8864	1227.1283	1230.0946
	H	-1.425110	-2.390382	-0.154144	1300.5796	1327.5570	1363.2140
	H	-3.442584	-0.994728	0.024605	1457.0780	1490.4631	1537.6625
	H	-3.224787	1.478915	0.182736	1638.2974	1674.5943	1729.7569
	H	-0.975397	2.505912	0.133794	2237.7773	3150.2992	3172.9073
	H	0.849998	-2.640599	-0.658350	3185.1682	3197.5316	3208.8754
	H	2.634189	-0.644335	0.831071	3220.3365	3265.2963	3486.3078
	H	3.056974	-2.329658	0.198126			
	H	3.235817	2.543378	-0.196288			
i8'	C	-0.284073	-0.567346	-0.026051	9.5161	130.8758	157.4544
	C	-1.520266	-1.223561	0.035671	236.6826	302.6369	386.0588
	C	-2.711452	-0.514456	0.059802	415.6795	439.8935	521.3724
	C	-2.691580	0.874075	0.018387	593.7658	637.7045	677.6956
	C	-1.473431	1.540753	-0.047964	703.4478	713.2157	742.9896
	C	-0.280953	0.832745	-0.070066	756.2174	807.3126	817.9282
	C	2.801687	0.232336	0.027092	867.9629	951.4372	977.9505
	C	3.361580	1.295647	0.072870	1001.3790	1014.7428	1025.2766
	C	0.923906	-1.399058	-0.044923	1025.8576	1067.1665	1125.9636
	C	2.224460	-1.066502	-0.024682	1190.3323	1217.4299	1224.5202
	H	-1.542473	-2.308341	0.066761	1279.0297	1350.8943	1372.9468
	H	-3.655079	-1.045651	0.109695	1448.0174	1496.5571	1546.0707
	H	-3.619682	1.434020	0.035840	1650.8503	1681.9915	1708.1809
	H	-1.450828	2.624104	-0.083898	2228.5258	3160.8780	3179.8972
	H	0.656094	1.369037	-0.124659	3182.5019	3190.3160	3201.7016
	H	3.844873	2.241835	0.114408	3214.3525	3244.2547	3485.0322
	H	0.720175	-2.466396	-0.074722			
	H	2.947650	-1.876409	-0.044235			
i10'	C	-0.039179	-0.598529	-0.087223	149.2787	193.5029	319.8048
	C	1.049679	-1.462697	-0.029810	352.5649	414.5719	468.0670
	C	2.323124	-0.924404	0.090133	532.6538	571.8877	602.8843
	C	2.518038	0.460815	0.127405	700.3799	711.4477	768.0919
	C	1.447195	1.334196	0.028787	778.7443	820.1708	836.2889
	C	0.161924	0.804297	-0.104074	876.0652	884.6465	909.7018

	C	-1.473187	-0.863571	-0.327379	975.9655	990.4584	1008.2570
	C	-2.740992	-0.449908	0.547062	1013.7019	1040.1141	1051.7224
	C	-2.073521	0.478668	-0.347874	1080.6972	1116.6729	1143.3067
	C	-1.147548	1.442872	-0.130992	1181.5395	1202.5783	1238.8308
	H	0.905598	-2.537436	-0.053520	1251.1796	1325.2973	1337.4936
	H	3.180313	-1.584044	0.166095	1376.8357	1477.9664	1495.6592
	H	3.524094	0.853046	0.226213	1513.5995	1632.8487	1651.5593
	H	1.605233	2.407017	0.042275	1680.8166	3114.7659	3176.2744
	H	-1.343172	2.445870	0.227755	3183.2298	3191.3704	3201.6365
	H	-1.741398	-1.622044	-1.055332	3207.3787	3212.2335	3213.6617
	H	-3.609267	-1.020353	0.232527			
	H	-2.674599	-0.272492	1.617774			
i14'	C	-0.551496	-0.745804	0.000119	160.4578	170.1678	317.4108
	C	0.549779	-1.588465	0.000037	340.9904	413.4474	432.3792
	C	1.901557	-1.261197	-0.000076	491.1917	582.0550	619.6338
	C	2.489649	-0.000176	-0.000111	690.5239	707.2044	726.0050
	C	1.901468	1.261143	-0.000004	750.4627	792.6176	809.5948
	C	0.550018	1.588576	0.000070	840.3741	890.5943	918.4208
	C	-1.892939	-1.145217	0.000124	960.5401	968.1179	976.4381
	C	-2.694215	-0.000082	-0.000108	993.4957	1013.0895	1030.3079
	C	-1.892740	1.145275	-0.000071	1075.0780	1091.7779	1184.9689
	C	-0.551672	0.745980	0.000125	1233.5111	1259.8397	1319.1221
	H	0.319486	-2.651795	0.000102	1330.4644	1334.5734	1438.4739
	H	2.589861	-2.100554	-0.000215	1445.4994	1502.2528	1510.3880
	H	3.576508	-0.000079	-0.000139	1557.1269	1607.6078	1673.9371
	H	2.589970	2.100339	0.000188	1680.9171	3154.3689	3157.0608
	H	0.319904	2.651927	0.000136	3164.4890	3183.7336	3192.6611
	H	-2.237760	-2.169905	0.000017	3217.0150	3235.4720	3245.0134
	H	-3.776703	0.000076	-0.000514			
	H	-2.237713	2.169794	-0.000207			
i15'	C	-0.000000	0.710436	-0.000014	172.3882	187.5683	371.2436
	C	-1.240994	1.396149	-0.000024	397.0018	482.7945	491.8846
	C	-2.422151	0.706504	-0.000003	524.2038	524.4771	638.8279
	C	-2.422142	-0.706495	0.000027	642.3857	737.1974	786.6656
	C	-1.240993	-1.396153	0.000044	795.4423	810.2756	814.7193
	C	0.000011	-0.710462	0.000026	861.3731	909.5643	956.8974
	C	1.240964	1.396132	-0.000052	979.5817	997.1913	1014.4181
	C	2.422157	0.706490	-0.000044	1020.1933	1046.0484	1060.7027
	C	2.422167	-0.706471	0.000001	1162.7515	1166.2657	1183.5364
	C	1.240983	-1.396134	0.000041	1196.7252	1239.8599	1277.5557
	H	-1.238442	2.481383	-0.000061	1298.4875	1402.8446	1425.2101
	H	-3.364627	1.242237	-0.000022	1432.7272	1503.5901	1507.3895
	H	-3.364609	-1.242248	0.000037	1572.3878	1655.1156	1674.2965
	H	-1.238486	-2.481387	0.000066	1716.8924	3179.9610	3180.6986
	H	1.238501	-2.481371	0.000059	3183.9097	3186.1099	3199.1521
	H	1.238468	2.481367	-0.000066	3199.7900	3212.4689	3213.3827
	H	3.364584	1.242310	-0.000045			
	H	3.364603	-1.242273	0.000014			
i13'	C	-0.012997	0.675396	-0.000021	101.5112	164.2787	243.6811
	C	-1.242515	1.389429	0.000020	355.2546	389.6346	447.1333
	C	-2.447858	0.726592	0.000194	491.1776	508.7660	550.3780
	C	-2.492591	-0.675524	0.000104	611.6950	663.7467	687.1800
	C	-1.313071	-1.407475	-0.000204	752.7432	761.4588	771.4022
	C	-0.079464	-0.763558	-0.000150	778.4302	872.5963	896.1741
	C	1.226036	1.319542	-0.000267	923.5604	927.2663	965.7384
	C	2.537849	0.603393	0.000089	997.2378	1045.8381	1062.1866

	C	2.396219	-0.904332	0.000163	1132.5867	1163.3102	1171.8118
	C	1.186919	-1.432916	-0.000139	1180.0962	1215.2821	1289.1676
	H	-1.213683	2.474199	-0.000154	1323.2037	1330.3082	1351.9090
	H	-3.372611	1.292660	0.000337	1428.0671	1450.9696	1453.3912
	H	-3.447696	-1.187080	0.000403	1509.7532	1583.2041	1628.8873
	H	-1.339596	-2.491142	-0.000405	1694.4065	2975.0817	2986.0842
	H	1.248495	2.404637	-0.000595	3175.8847	3180.9693	3184.1114
	H	3.137389	0.914796	-0.870127	3194.3400	3202.9490	3216.8332
	H	3.136554	0.914546	0.871016			
	H	3.299997	-1.505888	0.000792			
ts_i3' i4'	C	-0.000108	0.793129	0.095208	-402.7032	104.2766	132.0614
	C	-1.286652	1.394060	0.013752	142.8509	239.6456	299.9096
	C	-2.402796	0.626283	-0.118101	385.9842	394.3456	467.6403
	C	-2.349066	-0.809899	-0.167674	493.5832	534.3387	585.5143
	C	-1.175226	-1.446285	-0.013183	620.0197	669.1749	743.7067
	C	0.063438	-0.691426	0.338879	769.0282	830.6715	846.4508
	C	1.192368	1.514432	0.135327	886.1217	996.1587	1003.3038
	C	2.408481	1.019433	-0.292229	1010.2837	1021.3061	1033.6699
	C	2.539214	-1.672687	-0.102618	1069.5351	1082.1122	1148.9687
	C	1.363010	-1.290118	0.069820	1175.7606	1197.1737	1229.4115
	H	-1.357807	2.474528	-0.042092	1255.0524	1279.4053	1357.6108
	H	-3.364854	1.111750	-0.243126	1417.1199	1471.5034	1517.7014
	H	-3.258338	-1.365612	-0.361073	1538.5922	1607.0224	1696.3845
	H	-1.096073	-2.525142	-0.058452	2048.1177	2829.2723	3154.3032
	H	-0.023918	-0.670580	1.454016			
	H	1.163207	2.505553	0.582894			
	H	2.499656	0.336354	-1.116819			
	H	3.322137	1.511617	0.029568			
ts_i1' i4'	C	-0.091123	0.866899	-0.186334	-343.2872	83.7458	134.7632
	C	1.110215	1.459167	0.216361	189.9555	233.6230	300.1936
	C	2.257666	0.707781	0.328813	372.2704	426.5796	460.0669
	C	2.287346	-0.686148	0.043663	530.1334	567.7201	577.7212
	C	1.189907	-1.307218	-0.446177	634.8937	687.0968	740.8730
	C	-0.101352	-0.582499	-0.637257	776.5300	871.0067	896.9209
	C	-1.353533	1.444427	-0.011790	913.4959	976.5101	989.2745
	C	-2.481872	0.713608	-0.297829	1003.2138	1017.0532	1021.1109
	C	-1.894550	-1.782219	1.026892	1026.7958	1071.9580	1181.2312
	C	-1.074382	-1.298448	0.200042	1196.4786	1232.8921	1247.5370
	H	1.114589	2.503970	0.507281	1300.6707	1307.5716	1378.9353
	H	3.167136	1.185364	0.677011	1421.0562	1448.8600	1479.3157
	H	3.205990	-1.237875	0.202515	1544.5120	1599.4786	1655.4216
	H	1.200774	-2.357170	-0.711843	1972.4838	2937.1586	3178.2491
	H	-0.388494	-0.626239	-1.703222	3188.7105	3191.8965	3201.8685
	H	-1.431360	2.366006	0.555277	3211.4433	3226.8166	3271.4816
	H	-2.519865	-0.036133	-1.075746			
	H	-3.438701	0.989980	0.130428			
ts_i2' i4'	C	0.060409	0.768684	-0.060648	-195.3449	162.3753	217.6722
	C	1.293696	1.375806	0.114914	324.1885	389.7152	409.6334
	C	2.430318	0.568016	0.139852	479.6260	547.0982	582.5300
	C	2.319404	-0.810083	-0.000826	614.0870	739.2133	762.7328
	C	1.073649	-1.424222	-0.171251	774.5061	799.5455	832.3536
	C	-0.051502	-0.628800	-0.210053	858.4353	885.5481	909.4899
	C	-1.273656	1.346687	-0.171461	945.8131	962.3122	977.4715
	C	-2.217940	0.386515	-0.409220	1003.7090	1015.8533	1051.1334
	C	-2.269846	-0.697915	0.994525	1061.0557	1100.2382	1137.0512
	C	-1.509423	-0.960468	-0.247912	1187.8666	1191.3200	1194.3006

	H	1.376988	2.452413	0.214891	1234.4571	1267.1948	1327.7745
	H	3.408105	1.017891	0.265539	1347.9482	1395.0097	1484.1930
	H	3.215014	-1.420844	0.021668	1501.2903	1548.7940	1661.8304
	H	1.001585	-2.500985	-0.274312	1683.2726	3026.8742	3144.2771
	H	-1.464701	2.414367	-0.168629	3187.9813	3195.6411	3205.3429
	H	-3.219739	0.545827	-0.771970	3208.2852	3216.5075	3270.0326
	H	-1.568235	-0.306572	1.747568			
	H	-1.879671	-1.747413	-0.902263			
ts_i1'_i7'	C	-0.289240	-0.882490	0.456599	-1256.5825	137.3333	194.6650
	C	0.649608	-1.557886	-0.223108	256.6856	320.4520	346.0774
	C	1.973346	-0.968959	-0.435786	384.0703	454.3174	529.3166
	C	2.206183	0.332337	-0.217945	565.6620	583.9418	606.5859
	C	1.170572	1.200371	0.420791	613.9115	715.1459	722.6249
	C	0.014423	0.442245	1.020284	733.1309	774.2964	826.1883
	C	-1.170949	1.503661	-0.967698	868.5246	904.4808	929.8249
	C	-0.206741	1.374697	-0.122512	944.2587	965.2726	991.0144
	H	0.395165	-2.469106	-0.754617	1011.0435	1035.9183	1038.3692
	H	2.757961	-1.592391	-0.850188	1082.9443	1135.4506	1178.1817
	H	3.181378	0.763886	-0.412263	1210.6304	1260.4868	1303.7402
	H	1.545334	2.038676	0.998620	1363.4489	1407.0342	1431.4109
	H	-0.418571	0.726637	1.974531	1616.5025	1657.4391	1721.1870
	C	-1.760341	-1.072832	0.296589	1796.8473	2829.0236	3125.1118
	C	-2.497507	-0.097897	-0.222022	3159.7341	3168.8386	3172.5453
	H	-2.215930	-2.021379	0.579325	3182.0471	3192.1302	3210.8383
	H	-2.218133	1.104276	-1.146843			
	H	-3.563329	-0.190081	-0.419715			
ts_i2'_i8'	C	-0.238814	-0.567729	-0.040849	-918.7195	67.6465	122.6727
	C	-1.471328	-1.252248	0.043342	141.1714	220.1412	265.0335
	C	-2.664207	-0.561235	0.075594	356.3901	382.1393	412.4797
	C	-2.656624	0.833179	0.025064	504.5281	524.0698	605.6989
	C	-1.455115	1.524266	-0.060756	632.4815	703.6260	734.3944
	C	-0.248651	0.840926	-0.095599	785.8096	807.5755	872.6792
	C	2.794711	0.402138	-0.093138	932.7628	946.3124	979.0773
	C	3.221510	1.560113	0.150669	1019.5608	1019.8615	1044.5098
	C	0.954569	-1.358339	-0.081396	1061.0442	1129.0694	1172.8741
	C	2.297158	-0.954139	-0.051888	1194.9833	1205.6132	1222.0738
	H	-1.473043	-2.336796	0.081117	1266.3920	1369.0422	1371.1710
	H	-3.602604	-1.098849	0.139861	1435.3016	1480.5167	1528.1619
	H	-3.593547	1.378039	0.051356	1572.4187	1639.1983	1671.9971
	H	-1.453065	2.606788	-0.102795	2004.6959	2506.8891	3138.1032
	H	0.684805	1.383777	-0.163588	3177.6071	3187.1129	3197.4084
	H	2.408913	-0.552690	1.053246	3211.4689	3219.7622	3228.5579
	H	0.801739	-2.434543	-0.084173			
	H	3.027546	-1.747324	-0.201275			
ts_i3'_i6'	C	-0.037439	-0.773514	0.017794	-701.3487	94.0723	128.3796
	C	1.222623	-1.387665	0.004914	142.8029	204.2809	289.5848
	C	2.396288	-0.664910	-0.035437	292.7525	394.6198	411.9720
	C	2.383128	0.741518	-0.047092	464.8625	498.8621	543.5582
	C	1.190133	1.398382	-0.013986	600.8425	626.5397	689.9112
	C	-0.079747	0.686747	0.067267	735.4930	792.3423	828.4636
	C	-1.204107	-1.636109	0.030985	853.9912	914.1417	1014.2681
	C	-2.495216	-1.288485	-0.067760	1031.9236	1037.0965	1039.7209
	C	-2.345516	2.142008	-0.006478	1054.5760	1060.5737	1135.0302
	C	-1.304282	1.452618	-0.103216	1177.0231	1201.1970	1229.1260
	H	1.265517	-2.471190	0.001061	1272.6206	1348.2405	1388.8583
	H	3.343868	-1.191187	-0.056209	1437.0790	1472.0452	1496.7900

	H	3.312649	1.295700	-0.086482	1571.6188	1671.6477	1682.1564
	H	1.133342	2.480118	-0.008561	2024.2363	2642.7845	3150.4886
	H	-0.378288	0.885843	1.166950	3162.4013	3193.2215	3206.8765
	H	-0.962948	-2.693176	0.117321	3216.4617	3229.5900	3266.0577
	H	-2.820439	-0.261020	-0.166350			
	H	-3.248896	-2.068633	-0.049679			
ts_i4'_i5'	C	-0.072260	0.812840	0.189983	-346.9839	92.7687	147.8511
	C	-1.420299	1.361658	0.150233	228.8748	292.9536	369.6832
	C	-2.446650	0.527191	-0.081900	455.1677	490.8333	511.3562
	C	-2.225558	-0.901036	-0.322946	572.3296	617.4132	666.9525
	C	-1.045061	-1.477537	-0.083599	687.2930	707.8875	787.7275
	C	0.050499	-0.657409	0.555561	842.7598	849.9934	896.0333
	C	1.076594	1.402012	-0.134307	923.1471	974.7181	999.3337
	C	2.360147	0.610120	-0.222634	1009.2331	1010.6888	1026.7970
	H	-1.567071	2.432975	0.229209	1096.7403	1165.2422	1173.0880
	H	-3.456546	0.913112	-0.161984	1192.6482	1199.9218	1246.3686
	H	-3.048280	-1.487487	-0.716172	1263.3878	1324.1236	1348.7647
	H	-0.873808	-2.532260	-0.262043	1402.6561	1447.8936	1475.3786
	H	-0.060002	-0.755264	1.648210	1647.1159	1710.1537	1762.3162
	H	1.140379	2.457625	-0.381408	2047.3829	2970.1712	3090.4979
	H	2.800557	0.758028	-1.207838	3151.8860	3184.4319	3187.7609
	H	3.070924	0.934504	0.537864	3195.6023	3210.8374	3219.0333
	C	2.621072	-1.176519	-0.166958			
	C	1.433822	-0.954859	0.168927			
ts_i4'_i11'	C	-0.031324	0.870880	0.146631	-1072.2090	144.7430	148.1381
	C	-1.374437	1.388100	-0.031192	276.0142	370.4362	398.7509
	C	-2.388239	0.517599	-0.189438	474.4897	513.3518	529.0499
	C	-2.170366	-0.930240	-0.213914	567.2073	657.9017	685.6666
	C	-0.994838	-1.467244	0.126308	727.2174	734.0441	792.6608
	C	0.092595	-0.577778	0.652822	839.1264	868.3845	887.3777
	C	1.163215	1.434978	-0.118171	932.0923	971.4455	999.3815
	C	2.241146	0.443423	0.137457	1005.3318	1014.0374	1026.7392
	C	2.186549	-1.134183	-0.823928	1091.9802	1110.9186	1166.2693
	C	1.505513	-0.824030	0.267465	1181.3419	1183.5055	1215.5738
	H	-1.534125	2.457469	-0.114647	1243.1017	1279.0740	1312.3725
	H	-3.392471	0.885860	-0.368928	1343.0553	1400.3490	1449.8325
	H	-2.989214	-1.564028	-0.535342	1635.2690	1655.0181	1724.2306
	H	-0.827494	-2.537854	0.103036	1728.3993	2236.8128	2972.9629
	H	-0.017907	-0.535777	1.749920	3152.0376	3183.9045	3192.7954
	H	1.315785	2.462066	-0.424393	3206.1641	3215.3548	3220.4298
	H	2.974685	-0.147868	-0.915156			
	H	3.091856	0.651099	0.781286			
ts_i7'_i9'	C	0.174138	0.894868	0.464856	-484.2464	166.0743	199.5441
	C	-0.798686	1.496948	-0.284803	271.7838	371.0854	398.9602
	C	-2.026931	0.816183	-0.518307	435.1074	523.3554	544.9389
	C	-2.184325	-0.486278	-0.155690	605.9680	630.0293	686.5277
	C	-1.133932	-1.154563	0.564245	719.1574	774.6107	799.1964
	C	-0.070165	-0.382968	1.037014	840.2617	867.1267	887.4390
	C	1.629093	-1.047215	-0.680090	928.4076	931.5897	987.7087
	C	0.421473	-1.604596	-0.484401	994.9547	1004.1122	1015.5534
	C	1.618969	1.183450	0.362241	1063.7570	1084.1080	1164.2602
	C	2.305696	0.179713	-0.204300	1194.4068	1199.6623	1211.1177
	H	-0.606728	2.445648	-0.772598	1241.7825	1335.6948	1387.4597
	H	-2.820873	1.326903	-1.052167	1422.7453	1458.3617	1495.1393
	H	-3.089073	-1.030144	-0.394237	1612.5571	1641.1341	1653.0312
	H	-1.340778	-2.117615	1.009382	1676.7640	3110.0942	3183.5105

	H	0.612677	-0.769356	1.782835	3190.2303	3206.0289	3213.0042
	H	2.192226	-1.636678	-1.407029	3215.7628	3221.4458	3237.8220
	H	2.072428	2.129147	0.632767			
	H	3.368139	0.278848	-0.403546			
ts_i5'_i10'	C	0.110734	0.649848	-0.023375	-1361.7781	136.6538	185.2998
	C	-1.079495	1.466771	-0.047476	252.7610	329.4579	389.9967
	C	-2.305849	0.897124	-0.002306	420.8475	471.6178	510.4305
	C	-2.485370	-0.531893	0.050122	554.5267	569.8485	613.1081
	C	-1.421157	-1.363225	0.056658	735.9339	745.5812	756.9589
	C	-0.087690	-0.811887	0.021271	819.4871	853.5861	867.1709
	C	1.384191	1.146578	-0.095351	935.6016	986.3634	1004.1784
	C	2.688368	0.374869	0.310684	1009.3356	1014.3951	1047.3277
	C	2.159442	-0.743977	-0.419938	1072.9235	1110.6759	1153.1397
	C	1.157288	-1.507853	-0.183957	1185.0962	1208.3747	1239.9737
	H	-0.974913	2.545000	-0.096380	1267.8103	1315.3367	1377.9091
	H	-3.187842	1.527996	-0.006423	1429.6611	1494.5211	1528.4882
	H	-3.490902	-0.934888	0.064152	1578.7487	1594.1497	1701.0740
	H	-1.534443	-2.441264	0.068586	1768.0083	2023.7810	2957.6145
	H	0.577787	-1.513172	0.983170	3119.9240	3184.6302	3187.1141
	H	1.524424	2.204858	-0.290970	3197.1312	3205.9750	3218.3873
	H	3.552553	0.878446	-0.121537			
	H	2.810571	0.274897	1.401401			
ts_i5'_i14'	C	0.155578	0.666209	0.065085	-1335.8982	116.2181	139.5281
	C	-1.064346	1.450055	-0.016417	273.0849	354.5921	417.3546
	C	-2.278960	0.880848	-0.078954	444.8115	471.9180	506.3818
	C	-2.448423	-0.567417	-0.100696	579.5135	609.6035	625.6464
	C	-1.412929	-1.382580	0.097259	705.2903	725.7933	754.8194
	C	-0.035473	-0.870865	0.421454	807.1137	825.3235	896.4460
	C	1.389974	1.242746	0.019770	925.3737	975.0167	1001.0289
	C	2.579148	0.419357	-0.016549	1010.2730	1018.1512	1034.6863
	C	2.280586	-0.951233	-0.245995	1084.3617	1105.3804	1168.1982
	C	1.031404	-1.231676	-0.491920	1174.2626	1207.7782	1229.7278
	H	-0.962875	2.529340	-0.063811	1241.5538	1319.2148	1363.1166
	H	-3.160293	1.506479	-0.164965	1389.9402	1414.4930	1461.8171
	H	-3.433217	-0.969881	-0.309267	1586.0812	1630.0905	1657.5034
	H	-1.529517	-2.459936	0.059248	1738.5659	2153.9122	2864.4588
	H	0.167257	-0.992695	1.506547	3180.9574	3188.3495	3191.2586
	H	1.472593	2.324500	0.039551	3203.9122	3213.7346	3216.1639
	H	3.580796	0.809590	0.114305			
	H	2.685890	-0.680064	0.900181			
ts_i5'_p7	C	0.092362	0.708793	-0.163319	-1774.1193	170.7525	212.4764
	C	-1.159431	1.413804	-0.205400	337.6866	396.2124	411.6183
	C	-2.331916	0.761045	-0.042985	444.6197	499.4983	531.1133
	C	-2.374582	-0.667148	0.145856	564.0932	597.5462	684.5975
	C	-1.250805	-1.410487	0.162145	732.3271	747.0833	810.2716
	C	0.054532	-0.777176	0.049840	837.4554	871.0246	888.0095
	C	1.314910	1.297842	-0.013502	993.0280	1001.1446	1007.2547
	C	2.412725	0.408583	0.370570	1019.4793	1030.1242	1089.9061
	C	2.316825	-0.801403	-0.392713	1102.4794	1140.9218	1145.2376
	C	1.236496	-1.359386	-0.525794	1189.7172	1231.1244	1246.7323
	H	-1.140219	2.487655	-0.357733	1279.2042	1319.0860	1328.2847
	H	-3.265199	1.311802	-0.062770	1359.7174	1415.7419	1429.5145
	H	-3.340773	-1.149171	0.244620	1492.7233	1544.0746	1601.9985
	H	-1.288041	-2.489379	0.251111	1610.5933	1717.1474	2116.6851
	H	0.734422	-0.648026	1.343992	3186.0049	3193.7080	3194.2480
	H	1.416294	2.370735	0.096684	3209.9044	3214.1618	3218.8253

	H	1.670945	-0.165891	1.454223			
	H	3.345885	0.835470	0.721684			
ts_i9'_i15'	C	0.045208	-0.710865	0.183656	-256.6632	113.1292	163.7679
	C	1.238037	-1.381809	-0.134859	305.9826	344.2974	420.1251
	C	2.414177	-0.676034	-0.277539	456.9248	476.7649	544.7564
	C	2.446731	0.715607	-0.094400	583.8789	630.0264	729.6151
	C	1.296351	1.389228	0.248335	736.8996	747.0403	804.0099
	C	0.097051	0.675748	0.382375	824.8732	853.8060	879.5748
	C	-2.453982	0.672845	-0.345164	930.2244	985.2741	990.2517
	C	-1.559111	1.670245	-0.237699	1009.9509	1022.7931	1029.7196
	C	-1.232798	-1.379210	0.254730	1052.3405	1114.8402	1161.4853
	C	-2.389317	-0.725893	0.017433	1181.7968	1190.4699	1205.3894
	H	1.220581	-2.456110	-0.285044	1253.1412	1307.0771	1374.0683
	H	3.325523	-1.200783	-0.541486	1439.1609	1475.2039	1524.4817
	H	3.378592	1.254339	-0.218838	1586.3251	1645.8445	1674.8366
	H	1.291437	2.460977	0.404956	1681.2487	2849.0155	3127.3168
	H	-0.692785	1.141028	1.014533	3183.3225	3186.2010	3199.2654
	H	-3.367641	1.030266	-0.823879	3203.4018	3210.5388	3223.3363
	H	-1.247214	-2.450602	0.425085			
	H	-3.322578	-1.278290	0.043459			
ts_i10'_i15'	C	-0.060892	-0.569248	-0.098861	-1191.3347	150.9267	187.2825
	C	0.990271	-1.466807	-0.034542	321.3644	354.8304	398.4059
	C	2.286310	-0.969246	0.082836	471.0144	531.5966	580.7645
	C	2.526977	0.404011	0.112707	597.7149	673.6980	707.0837
	C	1.479771	1.313188	0.024630	749.3246	777.2417	800.7306
	C	0.183640	0.819410	-0.089902	856.3133	870.2203	878.6112
	C	-1.523931	-0.774352	-0.359453	909.4243	973.3020	983.1338
	C	-2.629919	-0.794312	0.638416	1004.3166	1016.9666	1052.9029
	C	-2.102841	0.600230	-0.234707	1097.1003	1145.4722	1166.0379
	C	-1.108469	1.505621	-0.061920	1186.6805	1226.7361	1237.7154
	H	0.811315	-2.536024	-0.058746	1276.5419	1314.8157	1344.8931
	H	3.120647	-1.657845	0.154611	1405.5450	1438.6747	1494.0957
	H	3.545185	0.764816	0.204262	1506.7480	1575.9799	1650.6061
	H	1.669817	2.380503	0.048239	1680.8851	2333.9865	3073.2086
	H	-1.720902	-1.252412	-1.320656	3101.8571	3186.1341	3194.5255
	H	-3.538695	-1.154088	0.141555	3204.1143	3214.3700	3215.7918
	H	-2.892132	0.502414	0.731135			
	H	-1.240738	2.541668	0.224380			
ts_i11'_i15'	C	0.023348	0.815712	-0.158787	-412.3177	137.1268	143.0816
	C	1.327750	1.399184	0.080044	330.1179	360.8575	448.5958
	C	2.404957	0.607989	0.216595	462.4490	505.4145	533.4453
	C	2.282655	-0.849918	0.169507	550.5861	663.2575	667.2755
	C	1.133315	-1.459017	-0.132154	718.8474	765.2027	793.4910
	C	-0.068781	-0.651082	-0.556552	827.5306	854.8257	873.5964
	C	-1.188590	1.386404	-0.041363	901.6169	971.9698	995.9983
	C	-2.340649	0.493324	-0.103962	1003.1333	1011.6553	1022.0956
	C	-2.402061	-0.734020	0.637406	1076.2082	1145.6790	1180.2431
	C	-1.379189	-1.147989	-0.067498	1199.7606	1223.4600	1236.6338
	H	1.406281	2.475332	0.194178	1263.5967	1264.5675	1335.4875
	H	3.378517	1.037870	0.421957	1354.0875	1397.4034	1450.5931
	H	3.157182	-1.444447	0.411213	1645.3894	1673.9603	1730.2218
	H	1.051228	-2.539403	-0.146803	1744.4107	2974.5634	3112.2043
	H	-0.111838	-0.692289	-1.657487	3181.5125	3186.1841	3188.0416
	H	-1.335717	2.458561	0.043978	3200.0153	3207.0854	3214.5645
	H	-3.149880	-1.207492	1.260278			
	H	-3.152308	0.748340	-0.786729			

ts_i8'_i12'	C	-0.049712	0.680515	0.347224	-455.1685	155.4179	163.3673
	C	1.127833	1.419814	0.057456	286.5995	396.2744	419.4970
	C	2.298498	0.793832	-0.260797	461.9568	501.8278	516.0255
	C	2.380114	-0.625562	-0.266460	588.2675	617.2871	670.7905
	C	1.313526	-1.374567	0.112718	721.7259	740.3308	763.4229
	C	0.044129	-0.767210	0.451961	789.0467	825.5157	862.5791
	C	-2.388586	-0.685100	-0.373138	932.5765	976.9255	993.1484
	C	-1.465550	-1.538759	-0.144318	1011.5658	1034.3298	1076.7257
	C	-1.297829	1.338497	0.281488	1080.8256	1115.1813	1171.1732
	C	-2.406224	0.700833	-0.255885	1195.6510	1200.6144	1208.4446
	H	1.061484	2.502388	0.022367	1249.2321	1304.8572	1407.3089
	H	3.169665	1.379973	-0.529286	1429.6821	1444.2056	1503.5022
	H	3.314678	-1.104238	-0.536575	1506.8878	1590.5081	1686.7874
	H	1.396876	-2.453799	0.184859	1815.2209	3041.0874	3164.6031
	H	-1.458256	-2.574745	0.157744	3181.5716	3183.4567	3186.9811
	H	-1.295435	2.424612	0.322492	3201.2404	3214.1144	3258.9541
	H	-3.172692	1.307643	-0.727501			
	H	-0.353519	-1.135592	1.404408			
ts_i6'_i13'	C	-0.000036	0.682149	0.089140	-573.7902	145.9917	171.3806
	C	1.231316	1.380703	0.113501	330.4214	345.7897	402.2904
	C	2.432437	0.718568	0.065169	459.2099	492.8880	501.4963
	C	2.466916	-0.680123	-0.060469	563.1958	595.2604	635.1993
	C	1.294117	-1.396583	-0.089940	698.0839	724.8878	758.8764
	C	0.043533	-0.763264	0.046562	772.6437	795.8960	863.0307
	C	-1.220997	1.340878	-0.207637	894.0888	912.1290	990.8540
	C	-2.478803	0.792395	0.047151	1019.3898	1021.0258	1059.7236
	C	-2.382597	-1.059356	-0.030799	1071.3812	1115.2112	1146.6291
	C	-1.181310	-1.462582	0.018641	1192.2144	1247.2784	1253.9108
	H	1.212851	2.462216	0.194583	1261.1372	1302.0437	1329.2518
	H	3.359551	1.278819	0.109952	1441.1228	1479.1792	1493.8909
	H	3.418939	-1.193742	-0.127092	1548.6526	1603.2117	1677.4730
	H	1.307364	-2.476575	-0.170771	1843.9123	3077.0630	3157.6541
	H	-1.147255	2.226417	-0.832485	3177.3902	3185.1125	3197.0452
	H	-2.695423	0.557947	1.090912	3209.0311	3220.9526	3291.2606
	H	-3.326486	1.259275	-0.451066			
	H	-3.356991	-1.431070	0.238052			
ts_i13'_p2	C	0.001053	0.661444	-0.040435	-838.0298	158.1571	175.7368
	C	1.214982	1.393608	-0.029220	310.2395	354.5751	386.2769
	C	2.422017	0.749200	0.013325	416.0744	484.0704	505.3511
	C	2.481167	-0.660990	0.045579	518.2315	526.6650	620.4520
	C	1.330084	-1.404719	0.031759	631.3045	751.7741	775.3449
	C	0.069894	-0.766219	-0.013353	784.1710	802.8806	822.2828
	C	-1.265281	1.292898	-0.085581	861.8496	893.9686	934.6840
	C	-2.440248	0.560352	-0.041864	981.9007	1013.4015	1023.9287
	C	-2.385774	-0.873730	-0.078299	1028.6292	1052.7211	1142.7943
	C	-1.164879	-1.437227	-0.046468	1169.8531	1179.7815	1204.6026
	H	1.170131	2.477563	-0.051301	1238.7124	1276.2389	1372.3607
	H	3.342275	1.322015	0.024232	1383.3316	1403.9109	1453.7897
	H	3.444965	-1.155435	0.081294	1499.2042	1528.0391	1609.5431
	H	1.367506	-2.487480	0.054561	1648.0047	1688.6477	3189.5230
	H	-1.308789	2.375830	-0.120103	3191.5621	3201.2980	3202.5010
	H	-2.901578	0.778760	1.789636	3211.5120	3212.5072	3224.5301
	H	-3.391424	1.054515	-0.203439			
	H	-3.301177	-1.453480	-0.107529			
ts_i12'_p1	C	0.017349	0.733664	0.121772	-1150.4479	164.5210	177.0445
	C	1.242597	1.485828	-0.051545	354.3085	367.0502	451.0240

	C	2.388975	0.785616	-0.100631	476.7358	482.9481	519.2874
	C	2.515894	-0.606751	-0.054822	551.9536	560.2101	612.3225
	C	1.352771	-1.338675	-0.000914	631.4637	741.7192	744.6742
	C	0.087658	-0.704460	0.028837	770.1641	788.3096	809.9221
	C	-1.265212	1.361517	-0.042649	837.1618	898.9671	934.1447
	C	-2.400333	0.612077	-0.096281	963.1249	983.8709	1011.7818
	C	-2.333041	-0.803123	-0.035042	1039.6091	1050.8252	1138.8462
	C	-1.121562	-1.438226	0.011755	1160.1232	1180.0100	1207.8636
	H	0.005609	0.786139	1.830266	1250.1028	1273.6276	1329.8257
	H	1.201172	2.568857	-0.094271	1387.2447	1407.0406	1460.2728
	H	3.483661	-1.092840	-0.090231	1479.1700	1529.9327	1605.6053
	H	1.393480	-2.423599	-0.002085	1642.0211	1682.7680	3187.9442
	H	-1.308562	2.444233	-0.084164	3189.1044	3194.7325	3195.7067
	H	-3.365136	1.096249	-0.195050	3207.6640	3215.0958	3218.2026
	H	-3.249171	-1.381617	-0.060202			
	H	-1.071630	-2.522230	0.012856			
p2	C	-0.014954	-0.755955	-0.000015	168.9236	188.5587	365.0024
	C	1.225168	-1.406957	-0.000020	402.5583	467.9169	512.0050
	C	2.440051	-0.818179	-0.000001	512.9354	524.6901	620.2945
	C	2.465472	0.604238	0.000027	633.7261	740.2211	783.2378
	C	1.298646	1.318946	0.000033	787.6832	803.6442	804.8856
	C	0.034839	0.671217	0.000013	879.6095	908.4423	938.1715
	C	-1.271040	-1.412543	-0.000035	987.3426	998.7420	1019.7357
	C	-2.428979	-0.684583	-0.000028	1041.9600	1059.5356	1148.2738
	C	-2.386939	0.728085	-0.000001	1174.6080	1186.7534	1207.8386
	C	-1.188285	1.387591	0.000020	1241.0049	1279.9910	1382.3414
	H	3.363261	-1.386765	-0.000006	1392.1567	1407.6242	1467.1580
	H	3.421169	1.116814	0.000043	1499.2263	1543.5251	1621.0908
	H	1.324983	2.403453	0.000055	1669.7256	1707.8182	3182.7762
	H	-1.294000	-2.495942	-0.000056	3183.7036	3193.9017	3194.4126
	H	-3.387494	-1.190678	-0.000044	3206.3370	3207.8785	3217.1115
	H	-3.314214	1.289622	0.000004			
	H	-1.157591	2.472335	0.000041			
p1	C	-0.017737	0.739444	-0.000028	174.2725	192.9952	373.2175
	C	-1.231841	1.489465	-0.000058	389.3675	476.2088	490.6266
	C	-2.389585	0.795511	-0.000033	515.2753	524.7647	621.1024
	C	-2.516891	-0.593635	0.000011	630.3714	754.0095	765.9911
	C	-1.353168	-1.322845	0.000028	780.4699	799.5452	818.5018
	C	-0.086328	-0.681409	0.000023	857.1146	900.7737	941.5607
	C	1.252857	1.367554	-0.000039	978.2473	992.9894	1017.6140
	C	2.399768	0.621933	-0.000016	1048.7064	1060.5550	1148.3335
	C	2.334650	-0.789296	0.000036	1167.8757	1178.1709	1215.2346
	C	1.122568	-1.422787	0.000070	1255.8290	1288.7745	1350.2713
	H	-1.196597	2.574021	-0.000091	1398.7911	1424.4384	1471.3090
	H	-3.485373	-1.079747	0.000032	1484.2417	1553.3214	1631.3633
	H	-1.391450	-2.407884	0.000071	1656.1840	1699.9919	3180.3682
	H	1.300473	2.451432	-0.000077	3182.5817	3185.2704	3187.8972
	H	3.366181	1.113209	-0.000034	3201.0983	3206.1004	3213.9811
	H	3.251141	-1.368016	0.000053			
	H	1.069872	-2.506631	0.000101			
p3	C	0.454156	-0.726267	0.000056	163.0053	169.2581	297.3677
	C	-0.702059	-1.499759	0.000077	338.5211	403.5272	427.9253
	C	-2.038267	-1.111073	0.000036	476.2786	551.9568	601.7429
	C	-2.546214	0.190561	-0.000036	679.9803	690.6540	714.6692
	C	-1.795573	1.333193	-0.000093	764.3468	784.9115	820.5800
	C	-0.472005	1.678925	-0.000111	822.2191	880.7676	921.2191

	C	1.761089	-1.226630	-0.000101	951.7948	955.3936	962.6498
	C	2.650176	-0.147906	0.000085	994.9237	1009.5376	1076.2491
	C	1.945446	1.059928	0.000112	1090.8273	1152.8719	1227.9916
	C	0.579226	0.766838	-0.000042	1274.3128	1301.2565	1318.1798
	H	-0.528227	-2.573573	0.000067	1371.1734	1431.9351	1467.4251
	H	-2.772173	-1.910928	0.000046	1492.2002	1551.9484	1589.9293
	H	-3.628842	0.297633	-0.000058	1608.1375	1680.6304	3146.1456
	H	-0.212755	2.736432	-0.000071	3150.1974	3159.8468	3188.2061
	H	2.025807	-2.274684	-0.000198	3217.5904	3238.4053	3247.3685
	H	3.729282	-0.235025	0.000123			
	H	2.371053	2.053280	0.000187			
p6	C	-0.620947	0.681348	-0.000007	153.5736	170.5384	311.3108
	C	0.435512	1.575461	-0.000020	342.7581	412.2544	427.6730
	C	1.804225	1.316146	-0.000028	478.6595	537.6723	611.7948
	C	2.454688	0.087683	-0.000033	682.1005	705.0607	711.4669
	C	1.936316	-1.206068	-0.000027	748.3565	778.9220	825.0786
	C	0.606315	-1.606816	-0.000003	876.1622	913.8477	915.8863
	C	-1.982645	1.016260	0.000129	951.2027	972.8263	992.2363
	C	-2.744706	-0.162137	-0.000013	1011.0155	1029.8518	1066.1017
	C	-1.860337	-1.230846	-0.000029	1157.4987	1178.1062	1252.5288
	C	-0.534723	-0.818064	0.000016	1297.1510	1323.8290	1330.0582
	H	0.150697	2.625775	0.000016	1405.8380	1421.7279	1476.4999
	H	2.448783	2.189292	-0.000019	1499.5455	1524.3989	1600.4050
	H	3.540063	0.145052	-0.000046	1669.9403	1674.0020	3154.2611
	H	2.669657	-2.006016	-0.000052	3161.9296	3171.6624	3187.0859
	H	0.427352	-2.678789	-0.000031	3195.4696	3224.4831	3243.6418
	H	-2.374307	2.024610	0.000222			
	H	-3.824432	-0.217725	-0.000010			
p7	C	0.142455	0.608447	0.000331	169.9271	203.7917	376.5182
	C	-1.021435	1.414430	0.000019	406.5185	413.9333	436.4445
	C	-2.271920	0.851380	-0.000259	514.7264	523.0147	564.6586
	C	-2.430426	-0.548557	-0.000021	591.6241	707.5905	738.7483
	C	-1.335626	-1.375114	0.000114	773.8403	801.8927	827.1189
	C	-0.041058	-0.822494	0.000018	879.7225	893.5889	968.8923
	C	1.453037	1.191029	0.000358	991.1790	1021.4538	1053.2314
	C	2.614339	0.446027	-0.000547	1105.3929	1129.3842	1163.3595
	C	2.314743	-0.923352	0.000046	1190.6730	1230.3984	1256.8362
	C	1.211634	-1.462286	-0.000031	1334.7236	1359.6081	1414.3938
	H	-0.912736	2.493771	-0.000390	1444.0147	1493.9667	1553.6445
	H	-3.149484	1.487518	-0.000347	1603.4239	1691.5771	2107.0511
	H	-3.427659	-0.973367	0.000018	3185.3256	3189.1398	3197.1295
	H	-1.447952	-2.452270	0.000015	3210.1209	3221.1031	3229.2597
	H	1.524140	2.274226	0.000627			
	H	3.599232	0.893060	-0.000096			

Table S7. Cartesian coordinates and frequencies (cm⁻¹) of reactants, intermediates, transition states, and products of the reaction of the triplet dicarbon (C₂, a³Π_u) with styrene.

Structures	Coordinates			Frequencies (cm ⁻¹)			
Styrene	C	0.514046	-0.220422	-0.002888	35.3757	205.2452	235.4052
	C	-0.406082	-1.279246	0.000138	411.9531	446.3442	448.8429
	C	-1.778225	-1.044039	0.002937	561.4898	635.0096	655.4358
	C	-2.261384	0.261196	0.002283	710.5811	787.4429	798.7095
	C	-1.359664	1.326960	-0.001276	849.8200	927.6641	930.4721
	C	0.008594	1.090363	-0.003925	976.3294	998.8183	1014.9399
	C	1.953290	-0.528216	-0.004599	1030.0462	1040.1559	1056.1697
	C	2.972003	0.334803	0.006259	1111.8838	1182.6896	1205.3639
	H	-0.035896	-2.299492	0.000677	1226.7313	1318.0793	1345.5572
	H	-2.468403	-1.880365	0.005433	1362.6204	1452.0525	1483.2868
	H	-3.328938	0.449713	0.004174	1528.6315	1618.1117	1644.4888
	H	-1.727932	2.346982	-0.002467	1691.0547	3128.5909	3142.8072
	H	0.691241	1.932066	-0.007837	3157.0921	3163.5676	3173.4637
	H	2.185844	-1.590967	-0.015687	3182.0512	3190.6412	3221.9594
H	2.831819	1.409900	0.018921				
H	3.996802	-0.016229	0.003211				
C ₂	C	0.000000	0.000000	0.652837	1692.1597		
	C	0.000000	0.000000	-0.652837			
i16'	C	-0.226955	-0.474705	-0.156502	13.3830	58.5032	119.3364
	C	-1.325162	-1.268003	0.284322	203.1360	221.8871	311.5690
	C	-2.588564	-0.726806	0.431594	381.2556	407.8291	478.4133
	C	-2.816233	0.626082	0.154099	516.5446	553.9103	626.4390
	C	-1.753366	1.430033	-0.269116	666.4215	688.4084	768.6466
	C	-0.483769	0.899812	-0.422961	786.6703	826.7286	877.8561
	C	1.043550	-1.069367	-0.313803	899.2544	926.0891	972.4411
	C	2.273211	-0.353052	-0.805397	991.4895	993.2914	1036.8579
	C	3.076150	0.240545	0.267542	1058.1865	1111.9317	1176.9633
	C	3.439880	0.920747	1.254945	1189.7551	1198.7650	1246.0374
	H	-1.155307	-2.317093	0.502194	1293.9233	1330.0127	1354.3915
	H	-3.406735	-1.354751	0.766468	1409.6622	1430.4496	1481.4787
	H	-3.807068	1.048676	0.272041	1504.9827	1536.7128	1580.8538
	H	-1.921378	2.481604	-0.473593	1602.0058	2983.3962	3039.3098
	H	0.326624	1.549302	-0.730768	3159.8404	3167.1287	3172.6337
	H	1.168322	-2.103565	-0.013065	3177.1689	3186.9214	3194.2936
	H	2.031577	0.412340	-1.550911			
	H	2.931517	-1.068226	-1.320716			
i17'	C	-0.202060	-0.794745	-0.013099	67.5229	111.1136	138.2730
	C	0.957301	-1.459377	-0.393938	206.9851	221.4129	303.9405
	C	2.225363	-0.885072	-0.328909	331.7829	386.4066	440.5574
	C	2.388702	0.434588	0.187219	473.2330	543.7836	557.7366
	C	1.323126	1.173579	0.572214	605.6574	658.3481	712.4379
	C	-0.099524	0.665110	0.436023	749.5025	800.1168	864.4925
	C	-1.463982	-1.483046	-0.002273	901.1719	934.5332	968.4672
	C	-2.659719	-1.001336	0.395164	982.4032	1001.4087	1007.4490
	C	-1.670262	2.481832	-0.781306	1011.7111	1054.5109	1129.2937
	C	-0.870935	1.585048	-0.412355	1154.3632	1184.2944	1204.3102
	H	0.861232	-2.485746	-0.735156	1256.3089	1288.8988	1343.8265
	H	3.093033	-1.452030	-0.642106	1372.2512	1409.2403	1461.4630
	H	3.387146	0.848575	0.278517	1509.5024	1571.9417	1610.3885
	H	1.437594	2.180322	0.955319	1621.1608	2881.6074	3129.7388
	H	-0.585569	0.738077	1.428921	3153.0478	3155.2862	3165.3342
	H	-1.418269	-2.515629	-0.341807	3189.3766	3197.0433	3236.5931

	H	-2.803181	0.018713	0.728116			
	H	-3.540040	-1.631781	0.375753			
i18'	C	0.093381	0.689463	0.172934	75.0350	157.9824	260.6368
	C	-1.153240	1.445319	0.129349	316.5200	373.2104	436.0104
	C	-2.335642	0.829723	-0.074578	467.1898	482.7706	502.2898
	C	-2.403676	-0.613136	-0.276344	588.6751	650.4022	695.0907
	C	-1.333474	-1.391682	-0.069949	721.7681	779.2958	825.5398
	C	-0.045730	-0.809843	0.478605	849.3137	877.8046	908.1636
	C	1.287430	1.264407	-0.052843	940.3005	974.5260	977.9825
	C	2.594911	0.510793	-0.155242	988.8935	1009.2465	1042.3187
	C	2.350806	-0.960426	-0.227265	1065.9649	1153.0400	1173.3101
	C	1.187308	-1.540063	0.035618	1185.8841	1205.2188	1237.5573
	H	-1.095203	2.527591	0.192367	1267.4493	1299.0653	1341.7923
	H	-3.247657	1.411087	-0.150432	1389.1847	1442.4087	1458.2100
	H	-3.341676	-1.048426	-0.603953	1598.1075	1657.6971	1694.2290
	H	-1.372605	-2.464652	-0.218401	1732.7624	2902.9823	2979.1032
	H	-0.113004	-0.906317	1.578371	3001.4013	3134.3066	3153.2425
	H	1.333380	2.339212	-0.211609	3161.4448	3179.3327	3187.5921
	H	3.244735	0.747157	0.700176			
	H	3.139589	0.847020	-1.048221			
i19'	C	0.039132	0.729893	0.148634	120.6921	153.6462	321.0480
	C	-1.187660	1.418982	0.054430	358.4642	438.7716	458.4347
	C	-2.382917	0.749726	-0.084129	479.6741	519.0055	545.4210
	C	-2.408769	-0.683078	-0.220713	604.5364	657.2849	688.3682
	C	-1.295753	-1.424601	-0.042914	736.9205	753.6570	787.6944
	C	-0.016804	-0.778950	0.433630	839.2556	872.2320	896.6713
	C	1.291904	1.348863	0.013249	923.7047	950.4449	975.8406
	C	2.464014	0.626247	-0.127252	992.5559	994.7213	1035.2952
	C	2.427324	-0.816441	-0.187719	1070.7254	1105.9360	1149.9528
	C	1.251796	-1.417923	0.016774	1170.1041	1211.6016	1223.4958
	H	-1.168557	2.504481	0.018733	1255.2743	1288.0420	1312.1385
	H	-3.306346	1.307080	-0.187854	1341.3496	1401.6725	1450.7777
	H	-3.339769	-1.162893	-0.503504	1488.6396	1508.3436	1613.1424
	H	-1.300699	-2.501282	-0.164782	1635.0168	2732.2428	3148.2796
	H	-0.043675	-0.862878	1.548685	3152.6764	3156.7040	3161.1547
	H	1.324085	2.432488	-0.049648	3182.7254	3183.0508	3190.4574
	H	3.331500	-1.370344	-0.419157			
	H	3.409871	1.137038	-0.266414			
i20'	C	0.042258	-0.688167	-0.000051	132.3884	182.2211	262.2853
	C	-1.176421	-1.430301	-0.000081	359.5857	380.2070	450.5276
	C	-2.400609	-0.795816	-0.000010	488.1195	504.4365	533.3548
	C	-2.474601	0.607865	0.000060	610.0964	687.8184	724.6937
	C	-1.305153	1.363734	0.000061	746.1697	760.1206	764.3559
	C	-0.051558	0.751832	-0.000078	833.8189	869.4267	899.7585
	C	1.287165	-1.323422	0.000019	917.4995	933.3534	943.1675
	C	2.599104	-0.574616	0.000090	975.1638	1006.4529	1045.0504
	C	2.348379	0.878788	-0.000050	1134.2642	1162.6044	1166.4110
	C	1.191325	1.523500	-0.000053	1190.9779	1223.6955	1240.9228
	H	-1.123190	-2.513928	-0.000123	1290.5420	1330.5320	1339.6397
	H	-3.312320	-1.382849	0.000031	1414.6547	1445.6819	1451.2442
	H	-3.439557	1.101169	0.000204	1493.3641	1555.6858	1598.6284
	H	-1.361422	2.447593	0.000131	1666.3925	2941.0392	2943.4354
	H	1.128990	2.608377	-0.000188	3141.8415	3154.5261	3157.6607
	H	1.332304	-2.408103	0.000108	3161.9188	3174.9705	3189.1204
	H	3.208027	-0.866417	-0.871579			
	H	3.207832	-0.866221	0.871970			

i21'	C	-0.000086	-0.724288	0.000000	165.0086	165.4354	284.4940
	C	1.236291	-1.398833	-0.000024	361.1770	392.9350	478.8327
	C	2.484105	-0.680101	-0.000016	482.9604	506.2144	521.8829
	C	2.484098	0.680084	0.000017	598.7871	697.5755	699.0715
	C	1.236357	1.398789	0.000025	725.2810	741.7058	753.5172
	C	-0.000011	0.724311	0.000019	806.1708	809.9165	822.5273
	C	-1.236393	-1.398810	-0.000012	829.5772	849.3507	915.6279
	C	-2.484062	-0.680083	0.000101	942.8571	953.1859	953.2129
	C	-2.483996	0.680144	-0.000010	1054.5888	1055.1993	1125.3767
	C	-1.236326	1.398796	-0.000032	1183.6284	1199.2554	1209.7866
	H	1.245231	-2.483096	-0.000026	1286.8262	1360.8503	1393.2458
	H	3.414264	-1.236170	-0.000038	1412.8272	1429.6159	1455.3227
	H	3.414284	1.236113	0.000024	1474.1919	1475.9204	1535.3813
	H	1.245256	2.483058	0.000031	1645.1190	3163.2348	3166.5134
	H	-1.245254	-2.483072	-0.000035	3166.5860	3172.9885	3177.5162
	H	-3.414223	-1.236162	-0.000114	3179.6293	3192.5168	3194.5331
	H	-1.245264	2.483063	-0.000112			
	H	-3.414157	1.236220	-0.000137			
ts_i16'_i18'	C	-0.094670	-0.685730	0.296582	-434.5546	105.5546	120.5863
	C	0.978556	-1.435039	-0.148286	177.6657	264.3784	275.1609
	C	2.243388	-0.853449	-0.354361	378.9429	405.0940	499.5675
	C	2.451138	0.494721	-0.112002	506.1550	591.2962	603.4039
	C	1.413445	1.263719	0.396157	651.5819	715.7606	761.0391
	C	0.118661	0.722690	0.589709	790.0552	856.7493	898.2396
	C	-1.423958	-1.238454	0.320040	911.8173	947.8879	964.3958
	C	-2.617199	-0.357482	0.003962	1001.3803	1010.5100	1018.2302
	C	-2.037478	0.884770	-0.501351	1055.6050	1094.8337	1162.3686
	C	-1.095150	1.689901	-0.668436	1177.4754	1193.5323	1218.0527
	H	0.830807	-2.482969	-0.386281	1250.3753	1315.0271	1348.8040
	H	3.055268	-1.470868	-0.721478	1408.6355	1458.9825	1461.9438
	H	3.423140	0.939530	-0.286360	1518.8679	1579.1173	1603.3406
	H	1.572216	2.305170	0.647083	1865.6760	3014.5435	3067.3545
	H	-0.462017	1.162938	1.393871	3175.5293	3193.3532	3196.7045
	H	-1.544890	-2.315126	0.263926	3205.8084	3219.7489	3230.7238
	H	-3.246122	-0.182679	0.887642			
	H	-3.248798	-0.869887	-0.730487			
ts_i17'_i18'	C	-0.088967	-0.695312	0.171145	-348.4517	92.3213	149.5388
	C	1.032862	-1.432234	-0.150806	254.7500	255.9551	292.8032
	C	2.311958	-0.858632	-0.211458	377.4455	418.8473	443.9509
	C	2.474502	0.540226	-0.025839	503.9310	556.2341	564.2882
	C	1.413985	1.344527	0.248698	636.9463	689.3164	732.6695
	C	0.024677	0.803603	0.441950	744.9484	790.4147	851.3800
	C	-1.422763	-1.234458	0.037745	903.3098	928.0331	944.4754
	C	-2.583869	-0.585158	0.412075	973.0094	978.3148	1003.8891
	C	-2.275683	1.195005	-0.820862	1009.9657	1062.7916	1128.2578
	C	-1.083970	1.355614	-0.393131	1175.5383	1209.0876	1221.2262
	H	0.913110	-2.484186	-0.392160	1262.2602	1282.2187	1302.0368
	H	3.169524	-1.475672	-0.448419	1384.1772	1414.8671	1453.7008
	H	3.463494	0.974006	-0.125277	1518.8717	1559.2242	1594.9022
	H	1.544679	2.412685	0.377957	1715.0634	2894.0837	3145.2269
	H	-0.252523	1.012954	1.492268	3156.5168	3165.3164	3166.1076
	H	-1.510863	-2.162573	-0.521139	3185.2753	3197.8792	3250.7147
	H	-2.602269	0.130466	1.221609			
	H	-3.541540	-1.006762	0.138065			
ts_i18'_i20'	C	0.063272	0.692014	0.015167	-791.4144	100.4001	174.2491
	C	-1.161394	1.435703	-0.063342	261.2307	355.8234	393.7836

	C	-2.378332	0.810255	-0.056389	438.4837	453.3121	486.7596
	C	-2.470541	-0.608970	0.020946	502.2383	531.2690	663.4391
	C	-1.337832	-1.379060	0.084016	690.7904	704.4138	731.2922
	C	-0.040119	-0.779919	0.063169	752.3261	777.1115	832.9202
	C	1.298579	1.301884	0.024906	864.9501	886.5109	915.6519
	C	2.588123	0.526533	0.107823	962.0303	980.9389	993.0014
	C	2.354924	-0.909162	-0.202095	1012.3769	1025.5700	1139.6689
	C	1.227365	-1.598245	-0.225600	1151.4460	1179.8322	1209.6343
	H	-1.102171	2.517625	-0.120256	1233.1770	1296.5026	1335.4926
	H	-3.287456	1.397891	-0.112911	1384.9840	1410.4036	1434.5923
	H	-3.445847	-1.081506	0.010771	1484.6821	1534.4496	1596.5178
	H	-1.389166	-2.460851	0.123382	1624.3173	2167.2965	2903.7904
	H	0.628002	-1.292337	0.961244	2987.2232	3147.0245	3161.1507
	H	1.353561	2.384452	-0.048870	3173.7732	3185.0067	3194.9911
	H	3.027092	0.614554	1.119290			
	H	3.351712	0.973977	-0.544253			
ts_i18'_i19'	C	0.065248	0.718561	0.150647	-1311.4044	76.1138	154.7617
	C	-1.184529	1.435376	0.102769	302.5886	331.9139	415.4549
	C	-2.359031	0.778684	-0.070521	452.3789	467.8855	491.3912
	C	-2.408956	-0.663428	-0.232310	548.7746	586.1293	667.3158
	C	-1.310017	-1.414259	-0.054531	677.3312	700.8748	746.5645
	C	-0.013486	-0.793726	0.395884	788.4492	852.2211	855.9821
	C	1.275392	1.326152	-0.008149	882.6652	974.1801	982.0189
	C	2.489380	0.553010	-0.195120	983.7113	997.4180	1028.2960
	C	2.431762	-0.895466	-0.256926	1069.3038	1079.6056	1116.9833
	C	1.255296	-1.486066	0.019955	1154.6200	1172.5155	1193.5230
	H	-1.160075	2.520347	0.124100	1224.3946	1235.5458	1340.3726
	H	-3.281823	1.341980	-0.155800	1372.3292	1394.1894	1451.8977
	H	-3.350147	-1.122379	-0.514090	1471.8950	1568.3579	1596.6127
	H	-1.323790	-2.491952	-0.168394	1675.4205	2031.5946	2751.0667
	H	-0.045654	-0.891307	1.510206	3128.2376	3152.4894	3156.4189
	H	1.325641	2.407032	-0.100942	3166.3398	3180.7977	3191.4846
	H	3.006026	-0.188879	0.727590			
	H	3.383453	1.072135	-0.532852			
ts_i21'_i20'	C	0.038162	-0.697289	-0.030910	-1774.8683	162.8882	175.4299
	C	-1.171001	-1.418413	-0.013329	332.6514	368.6563	463.1116
	C	-2.400087	-0.771862	0.018090	490.3489	508.3748	510.2824
	C	-2.458239	0.623881	0.036186	585.6472	612.3925	632.5832
	C	-1.283616	1.367888	0.021754	673.8155	750.2210	758.8281
	C	-0.027455	0.741986	-0.018127	767.5898	782.5109	846.5422
	C	1.308320	-1.364199	-0.067097	866.1151	918.5556	932.3636
	C	2.500117	-0.618122	0.000483	972.7832	985.9451	1049.4181
	C	2.376226	0.806218	-0.013839	1055.9545	1109.9042	1137.9462
	C	1.200735	1.507803	-0.099924	1179.7150	1197.6917	1222.1538
	H	-1.130218	-2.502553	-0.024730	1246.6074	1271.8580	1310.2723
	H	-3.314897	-1.353552	0.031943	1371.9682	1408.1169	1431.5909
	H	-3.417079	1.128881	0.064546	1451.0567	1488.0668	1523.5434
	H	-1.327081	2.451792	0.036124	1588.7749	1603.3273	3157.1724
	H	1.352527	-2.445583	-0.027550	3162.4342	3174.0480	3176.4601
	H	3.477690	-1.080657	-0.069791	3187.8232	3188.0630	3191.0622
	H	2.690112	0.147545	1.169172			
	H	1.169980	2.586784	-0.179427			
ts_i19'_p2	C	0.037003	0.701195	0.040193	-1016.2530	168.0086	171.7085
	C	-1.189251	1.407886	0.011538	345.1139	381.2514	445.0832
	C	-2.391271	0.744251	-0.045852	471.2246	507.3598	517.3554
	C	-2.433568	-0.674328	-0.108567	544.2811	570.1877	610.1436

	C	-1.284713	-1.409675	-0.044190	631.1020	724.8624	745.0017
	C	-0.013935	-0.755716	0.142646	782.7127	788.2566	811.5759
	C	1.300758	1.337492	0.007352	864.4471	896.2739	925.7290
	C	2.472412	0.617159	-0.052196	960.1818	973.0127	994.1467
	C	2.444953	-0.809852	-0.107141	1024.9938	1037.1705	1134.0167
	C	1.235057	-1.403904	-0.039426	1160.1887	1170.9134	1194.6574
	H	-1.163032	2.492861	0.009720	1229.5262	1262.7214	1344.4693
	H	-3.317742	1.305797	-0.080697	1362.7239	1374.9686	1440.5896
	H	-3.389557	-1.173331	-0.219507	1474.4351	1512.2554	1559.1458
	H	-1.303617	-2.491674	-0.088980	1629.2336	1648.6441	3158.5081
	H	-0.017287	-0.837844	1.846494	3160.5562	3168.8533	3170.8291
	H	1.332913	2.421878	0.004905	3183.0449	3185.1733	3195.5525
	H	3.427999	1.128749	-0.087438			
	H	3.365647	-1.373483	-0.210633			
ts_i19'_i21'	C	0.000347	0.711711	0.026546	-1873.5427	145.0882	189.4323
	C	-1.207988	1.395783	0.014755	344.2882	381.5449	426.1275
	C	-2.427629	0.728088	-0.013875	488.3696	499.8014	521.4451
	C	-2.446272	-0.675424	-0.067159	588.6425	620.3022	651.1005
	C	-1.293037	-1.417279	-0.046922	722.6724	723.8358	771.7266
	C	-0.022806	-0.752026	0.088287	782.4608	797.6762	846.6123
	C	1.294307	1.347693	0.017265	914.0150	926.2344	947.3927
	C	2.456343	0.641302	-0.053322	982.0723	991.4840	1024.0739
	C	2.481299	-0.792151	-0.105453	1046.7890	1125.5905	1145.5293
	C	1.257122	-1.389643	0.010244	1172.8435	1189.0643	1229.5424
	H	-1.183535	2.481221	0.012238	1254.0872	1270.7046	1353.5791
	H	-3.356164	1.284316	-0.028913	1380.2537	1429.2959	1438.4848
	H	-3.397340	-1.190232	-0.152570	1465.5814	1507.4375	1557.4242
	H	-1.315131	-2.498033	-0.107105	1626.1567	1686.3152	3187.4175
	H	0.565979	-1.120621	1.256272	3189.3231	3193.9676	3209.3731
	H	1.326234	2.431813	0.025432	3218.8038	3226.2579	3236.2071
	H	3.402869	1.171396	-0.080383			
	H	3.406972	-1.348177	-0.147161			
ts_i20'_p1	C	0.051500	-0.671821	-0.040310	-843.7762	158.7911	185.4442
	C	-1.147686	-1.430452	-0.026697	309.7817	354.1646	381.7021
	C	-2.368399	-0.814199	0.018022	416.8788	473.4231	506.1157
	C	-2.452808	0.594820	0.048695	521.9764	524.9191	625.8557
	C	-1.314899	1.357746	0.030917	637.2487	748.9254	762.0406
	C	-0.038783	0.749881	-0.015678	777.1410	797.3110	835.5389
	C	1.320562	-1.295365	-0.088285	854.0098	893.1882	939.0503
	C	2.490903	-0.545578	-0.045002	979.8968	1003.1758	1012.2629
	C	2.333819	0.851709	-0.082502	1036.4164	1054.0546	1140.1751
	C	1.166466	1.520871	-0.050727	1165.3840	1172.6060	1213.8641
	H	-1.079086	-2.513098	-0.048687	1249.9620	1285.9356	1336.0081
	H	-3.276708	-1.405529	0.031140	1393.9117	1416.8195	1460.3533
	H	-3.425012	1.072857	0.085636	1479.2975	1541.0702	1603.8129
	H	-1.379266	2.440552	0.052127	1648.1407	1688.0196	3187.5546
	H	1.377048	-2.378281	-0.128075	3189.8616	3190.3897	3194.1244
	H	3.453941	-1.011899	-0.214980	3205.7917	3207.0808	3219.5828
	H	2.973944	-0.715014	1.789146			
	H	1.111088	2.604748	-0.056901			
ts_i21'_p2	C	-0.029893	-0.732597	-0.022282	-1032.0349	168.4611	179.5295
	C	0.002421	0.690953	0.028540	311.0563	359.2980	401.3655
	C	-1.269171	-1.405960	-0.068060	426.5881	475.8987	510.6143
	C	1.231514	-1.372818	0.018667	518.4235	537.3244	620.2440
	C	2.439849	0.664268	-0.067210	637.8109	738.0882	777.8497
	C	1.259482	1.356287	0.030550	788.0970	796.4201	805.4183

	C	-2.439610	-0.692769	-0.066579	875.5453	904.1807	933.1493
	C	-2.418313	0.716422	-0.001974	981.8276	992.3967	1015.8120
	C	-1.227598	1.391463	0.047982	1046.5149	1065.1446	1139.7585
	C	2.436561	-0.747849	-0.147660	1171.0887	1186.4229	1197.6172
	H	-1.276252	-2.488937	-0.101179	1241.5460	1276.4051	1370.5703
	H	1.307101	-1.579404	1.900763	1376.1162	1393.5562	1461.1417
	H	3.383578	1.196694	-0.108910	1488.4131	1531.5384	1606.2090
	H	1.269411	2.440351	0.069716	1643.5788	1692.3834	3190.3354
	H	-3.390208	-1.211846	-0.107332	3192.7114	3202.6504	3205.5776
	H	-3.353436	1.264499	0.010342	3214.4725	3217.4173	3225.6050
	H	-1.211170	2.475060	0.103431			
	H	3.359523	-1.300822	-0.278679			
ts_i18'_p8	C	0.072734	0.679213	0.113735	-622.0976	99.0528	174.7029
	C	-1.163172	1.426587	0.151486	254.7687	323.6407	356.8814
	C	-2.351918	0.800301	0.001067	392.9028	414.8975	458.7498
	C	-2.410160	-0.618592	-0.209300	477.6414	512.6414	571.6740
	C	-1.293416	-1.385350	-0.155489	585.3289	698.6506	736.2821
	C	-0.009530	-0.799291	0.124708	738.9269	772.2613	790.2706
	C	1.277562	1.272351	-0.108417	865.8409	886.9060	917.6105
	C	2.559793	0.513364	-0.177922	940.2287	1002.8511	1019.8503
	C	2.377685	-0.954017	0.004060	1025.8543	1032.0415	1124.3441
	C	1.208320	-1.500515	0.101751	1149.7910	1186.5000	1219.7333
	H	-1.115868	2.502017	0.286505	1270.9816	1292.5891	1302.1769
	H	-3.274455	1.368734	0.016036	1372.1178	1386.0905	1429.5508
	H	-3.372595	-1.079239	-0.401998	1492.0969	1588.9825	1609.5253
	H	-1.336270	-2.461423	-0.271869	1697.3127	2539.6664	2981.9634
	H	-0.151354	-0.919199	1.941560	3047.7639	3171.7330	3186.4938
	H	1.310353	2.343501	-0.290978	3195.7560	3211.8837	3220.6253
	H	3.173095	0.816766	0.689266			
	H	3.159712	0.824552	-1.042591			
ts_i21'_p1	C	-0.035556	-0.699478	-0.008459	-896.1883	167.2323	177.7696
	C	0.012951	0.734310	-0.037754	338.1752	355.8347	382.8869
	C	-1.298177	-1.363588	-0.062566	400.0538	482.0910	497.6016
	C	1.182356	-1.418893	0.036255	508.9111	527.1978	614.3787
	C	2.439063	0.647723	0.014386	628.3641	740.8145	751.6333
	C	1.276268	1.380109	-0.029875	768.3075	792.4280	803.2901
	C	-2.473858	-0.657358	-0.094209	840.0448	884.8755	933.0774
	C	-2.376833	0.747682	-0.003354	960.4058	972.9531	996.8780
	C	-1.210194	1.458817	-0.120495	1021.4194	1043.8391	1144.8397
	C	2.392831	-0.763280	0.050288	1160.8812	1171.0794	1207.7042
	H	-1.315586	-2.449001	-0.081024	1248.1206	1277.5640	1337.7659
	H	1.147986	-2.503042	0.058737	1377.3449	1387.8716	1441.9376
	H	3.398154	1.153125	0.025525	1460.6352	1526.1694	1571.1565
	H	1.309490	2.464044	-0.053883	1592.9018	1646.5630	3156.2044
	H	-3.434972	-1.157053	-0.125646	3161.1336	3163.7541	3166.9161
	H	-2.678177	0.886286	1.847006	3178.2274	3183.1742	3190.2171
	H	-1.196436	2.538860	-0.223280			
	H	3.316443	-1.329478	0.087263			
p1	C	-0.017603	0.744867	-0.000065	174.7110	191.9391	368.9068
	C	-0.086671	-0.686741	-0.000175	387.1416	471.8432	485.5325
	C	1.254921	1.371713	0.000237	511.3204	520.5914	611.1768
	C	-1.235908	1.492866	-0.000364	628.2606	744.9525	754.9233
	C	-2.524390	-0.593402	0.000310	767.3758	793.9531	805.9425
	C	-1.355353	-1.327170	0.000097	845.0879	887.9590	936.2458
	C	2.406862	0.622856	0.000267	956.7056	970.5860	996.6642
	C	2.342245	-0.789675	-0.000021	1039.9094	1049.6505	1141.2264

	C	1.125266	-1.426446	-0.000388	1161.1603	1172.2508	1208.0941
	C	-2.396147	0.795033	0.000061	1249.9930	1276.7413	1334.9347
	H	1.304086	2.455483	0.000216	1385.5716	1394.1306	1457.5025
	H	-1.202036	2.577588	-0.000727	1468.3565	1530.2587	1592.1810
	H	-3.492817	-1.080467	0.000048	1619.9673	1656.4690	3155.3312
	H	-1.394956	-2.412147	0.000721	3158.7415	3160.0078	3164.5357
	H	3.373165	1.114745	0.000279	3176.1842	3178.9532	3188.4097
	H	3.258959	-1.368331	0.000110			
	H	1.074266	-2.510282	-0.000404			
p2	C	-0.014294	-0.761883	-0.000017	168.0441	184.6911	363.0699
	C	0.035435	0.677500	0.000010	400.7015	466.6763	507.1903
	C	-1.273456	-1.416446	0.000010	512.2760	524.4624	619.3663
	C	1.226643	-1.409081	-0.000067	633.9413	732.3800	778.6348
	C	2.472983	0.604351	-0.000059	786.8410	798.7945	803.5742
	C	1.301611	1.322703	-0.000012	872.3706	903.3779	937.3431
	C	-2.435977	-0.685430	0.000060	980.4591	991.4903	1014.3854
	C	-2.394168	0.728826	0.000087	1041.2466	1058.0113	1148.5137
	C	-1.190851	1.391497	0.000064	1172.5475	1188.2692	1207.4658
	C	2.446291	-0.820206	-0.000092	1241.3544	1275.8201	1381.5534
	H	-1.296739	-2.499814	-0.000011	1390.7668	1406.4774	1465.4258
	H	3.369579	-1.389108	-0.000127	1500.0577	1542.8097	1620.9461
	H	3.429529	1.116099	-0.000073	1670.7290	1707.5307	3189.1218
	H	1.330351	2.407073	0.000012	3190.4639	3198.8112	3202.2413
	H	-3.394594	-1.191664	0.000079	3211.9321	3215.4344	3224.8483
	H	-3.321754	1.290095	0.000129			
	H	-1.161666	2.476341	0.000089			
p8	C	0.000000	0.618351	0.000000	139.8598	187.2873	242.8953
	C	-1.278220	1.237798	0.000000	350.7775	361.4956	406.8473
	C	-2.437706	0.490233	0.000000	443.1915	495.9068	541.3088
	C	-2.389770	-0.906885	0.000000	553.9759	635.9769	663.4773
	C	-1.161334	-1.563468	0.000000	732.3714	760.3119	766.7008
	C	0.015197	-0.838714	0.000000	854.6146	866.0412	910.9681
	C	1.179246	1.386252	0.000000	955.1827	968.2117	991.2943
	C	2.602989	0.829329	0.000000	1026.4837	1055.4076	1120.4450
	C	2.384292	-0.623960	0.000000	1154.1638	1166.0422	1189.9621
	C	1.377160	-1.299292	0.000000	1221.7637	1268.6378	1304.3734
	H	-1.335574	2.321032	0.000000	1326.4699	1397.4885	1442.2695
	H	-3.397720	0.993859	0.000000	1462.7997	1503.4722	1584.3055
	H	-3.308996	-1.480524	0.000000	1631.4432	2198.7733	3020.3746
	H	-1.114278	-2.645790	0.000000	3043.7948	3188.3353	3193.4253
	H	1.086922	2.467951	0.000000	3202.3124	3215.6947	3225.1280
	H	3.159260	1.182808	0.877632			
	H	3.159260	1.182808	-0.877632			

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