

Supplementary Materials for
**Gas-phase formation of the resonantly stabilized 1-indenyl ($C_9H_7^{\bullet}$) radical in
the interstellar medium**

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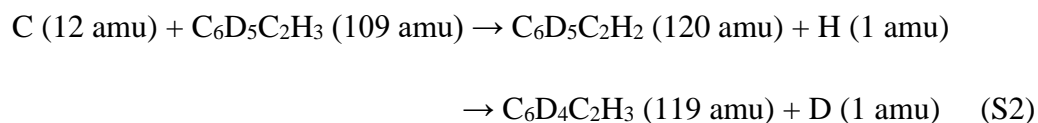
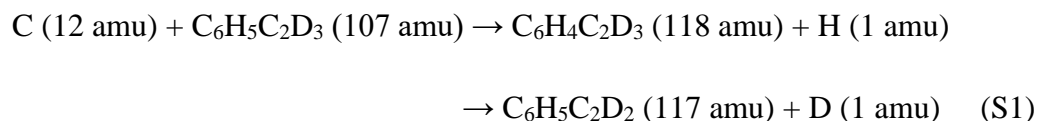
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Supplementary results

Since the atomic hydrogen can be eliminated from the vinyl moiety and/or the aromatic ring of the styrene, the reactions of carbon with D3- and D5-styrene were performed to trace the source. Signal was probed at m/z 118 ($C_9H_4D_3^+$) and 117 ($C_9H_3D_3^+/C_9H_5D_2^+$) in the C- $C_6H_5C_2D_3$ reaction (reaction S1) with the determined ratio of 0.89 ± 0.03 : 1 of 118 to 117 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- $C_6D_5C_2H_3$ system (reaction S2) the ratio of 0.74 ± 0.03 (120):1 (119) is calculated according to the same procedure. Meanwhile, the experimentally derived ratio of 118:120 is measured to be 1.18 ± 0.02 : 1 under the same experimental conditions of the secondary beam (pressure, pulse voltage, etc) and calibrated according to the intensity of the primary atomic carbon beam. Considering the four pathways i) **i2** \rightarrow **p3** + **H**, ii) **i2** \rightarrow **p2** + **H**, iii) **i6** \rightarrow **p2** + **H**, and iv) **i7** \rightarrow **p1** + **H** along with the RRKM-predicted ratios of 1-indenyl (iv: 54.7 %), 1-phenylpropargyl (ii: 29.5 %; iii: 12.1 %), and 3-phenylpropargyl (i: 3.5 %), the C/ $C_6H_5C_2D_3$ system (fig. S4) predicts that the signal from the atomic hydrogen loss (m/z 118, reaction S1) contribute 54.7 % since only pathway iv leads to the H elimination in this system. In the same procedure, the contribution from H loss in the C/ $C_6D_5C_2H_3$ system (m/z 120, reaction S2, fig. S5) is confirmed to be 45.1 % as the sum of pathway i-iii. Thus the RRKM- predicted ratio of 118 (H loss signal of C/ $C_6H_5C_2D_3$): 120 (H loss signal of C/ $C_6D_5C_2H_3$) should be 0.55 ± 0.01 : 0.45, i.e., 1.22 ± 0.03 : 1 under the same intensity of primary and secondary beam in the two systems. This ratio still holds with the existence of the fragmentation since the fragment ratio of 118 to 117 in C/ $C_6H_5C_2D_3$ system is also nearly the same compared to that of 120 to 119 in C/ $C_6D_5C_2H_3$ system. It should be noted that the dicarbon (C_2) and tricarbon (C_3) were also produced in the ablation source at minor levels of less than a few per cent. However, no signal from reactions of dicarbon or tricarbon was observed. Most important, signal recorded at m/z 115 can only be replicated with a single channel via reaction of atomic carbon with styrene.



The rate constants of the reactions included in the modeling are derived from the published results. For example, the rate constant for the reaction of atomic carbon with styrene is predicted according to the reaction of atomic carbon with stem compound ethylene which proceeds rapidly with the rate constant of $2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (45). As for the $\text{C}_3\text{H}_3\text{-C}_6\text{H}_5$ reaction, the rate constant is predicted to be a few $10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ under our experimental conditions (41).

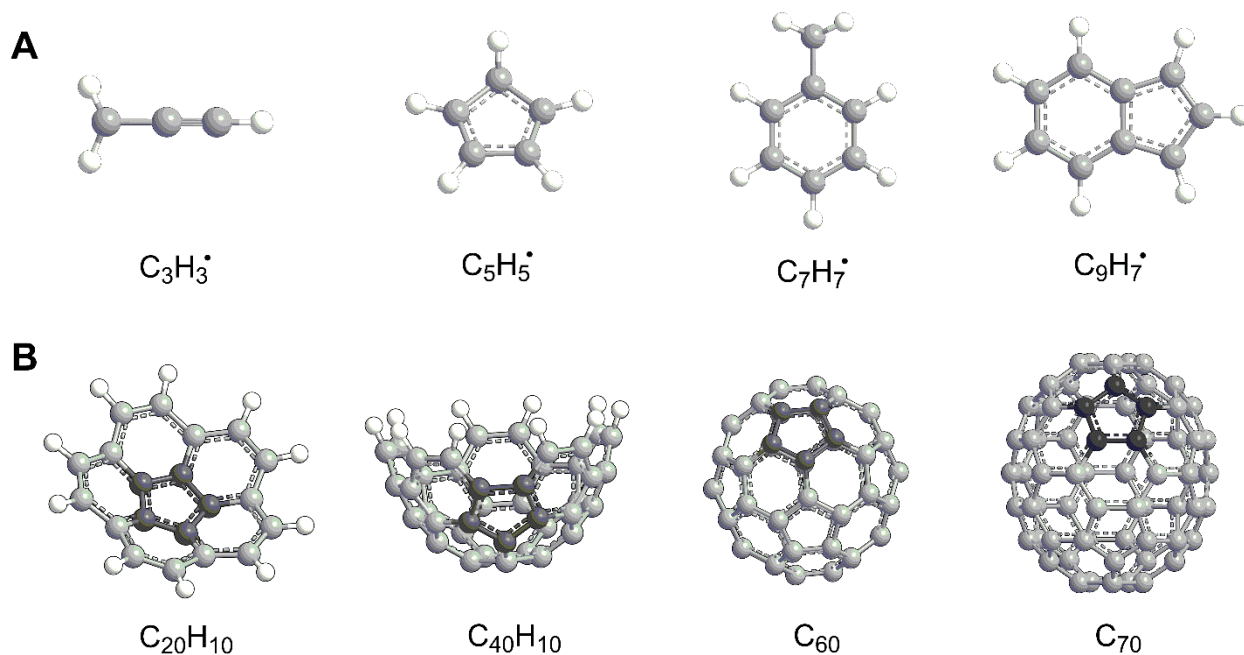


Fig. S1. Molecular structures of the selected molecules. Resonantly stabilized free radicals (RSFRs) (A) and corannulene ($C_{20}H_{10}$), the C_{40} nanobowl ($C_{40}H_{10}$), buckminsterfullerene (C_{60}), and rugbyballene (C_{70}) (B). Propargyl (X^2B_2), cyclopentadienyl (X^2E_1''), benzyl (X^2B_2), and 1-indenyl (X^2A_2) are key precursors to PAHs in both high-temperature and low-temperature molecular mass growth processes. Carbon and hydrogen are color-coded in gray and white, respectively. The carbon atoms of the five-membered ring are highlighted in black in (B).

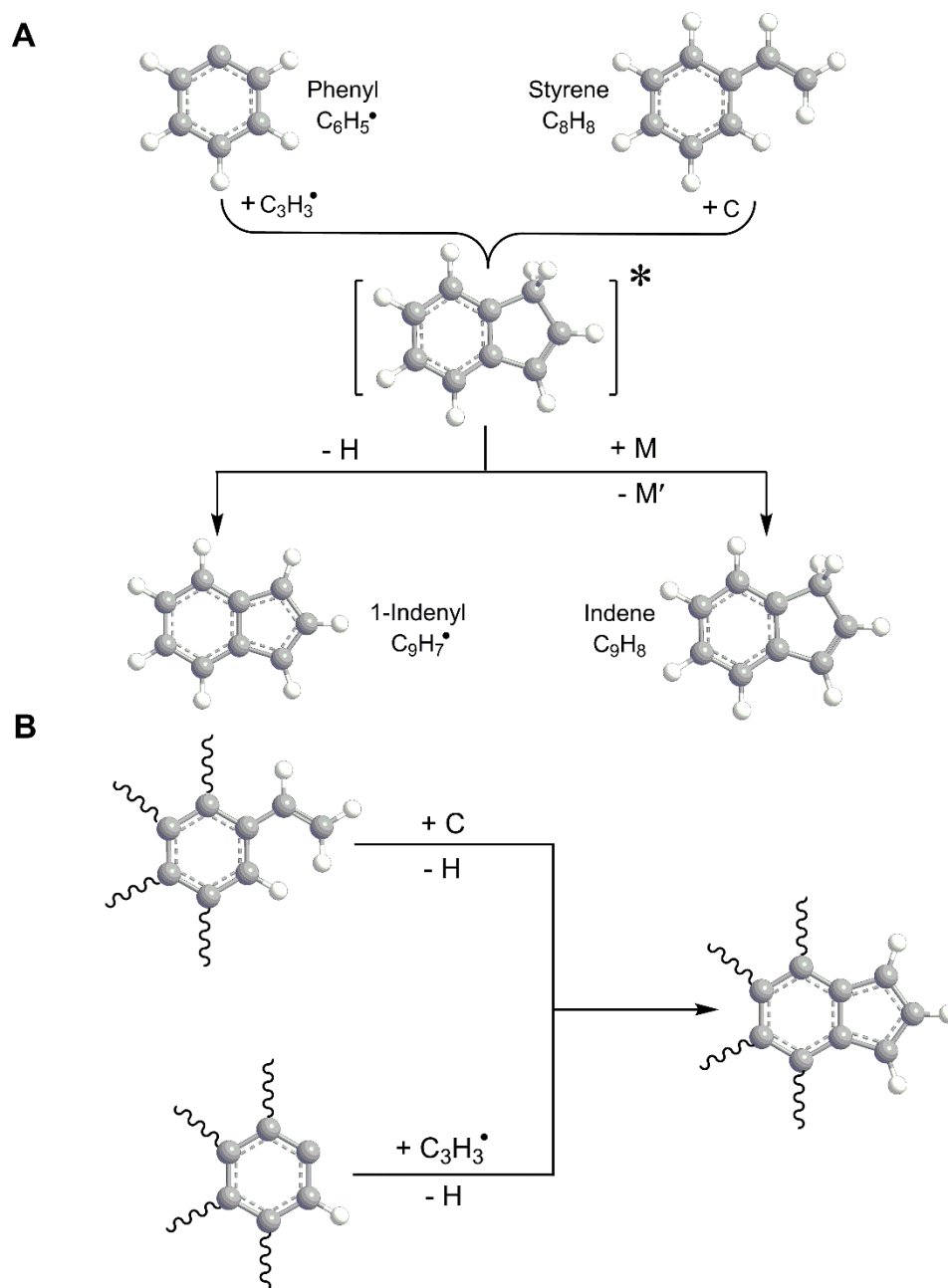


Fig. S2. Pathways to 1-indenyl and indene. Reactions of atomic carbon with styrene and propargyl with phenyl (A) and reactions involving more complex vinyl substituted or aryl radical reactants (B). Pathway to 1-indenyl ($C_9H_7^\bullet$) is opened under low-temperature single collision conditions while indene (C_9H_8) is formed at elevated pressures facilitating a three-body stabilization process within hydrocarbon-rich atmospheres like in Titan's atmosphere. The lower panel displays the broader impacts of our findings on molecular mass growth processes with the wavy lines indicating the incorporation within a PAH (B).

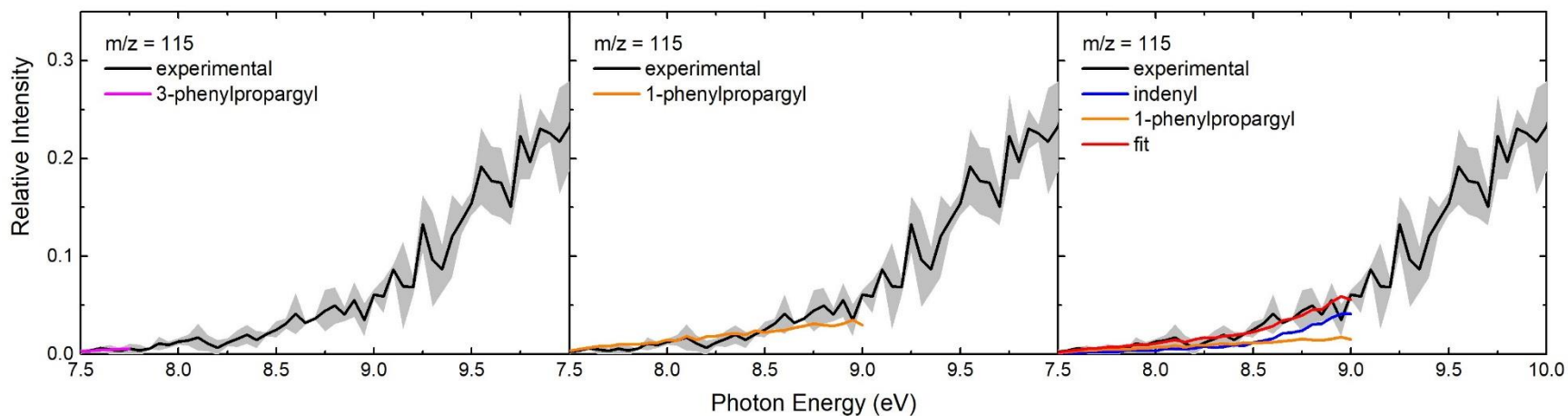


Fig. S3. The comparison of available experimental PIE of 1-phenylpropargyl (C_6H_5CHCCH) and 3-phenylpropargyl ($C_6H_5CCCH_2$) radicals with our experimental PIE curve of $m/z = 115$ along with the fitting of the PIE curve at 115 with the sum of two channels: indenyl and 1-phenylpropargyl in the photon energy range of 7.5 to 9.0 eV. Experimental PIE is collected from 7.5 to 10 eV while PIE of 1-phenylpropargyl and 3-phenylpropargyl are collected in a very short range 7.5 – 9.0 and 7.5 – 7.8 eV, respectively. More PIE data of reference radicals are needed to accurately calculate the branching ratios of the ion counts at 115.

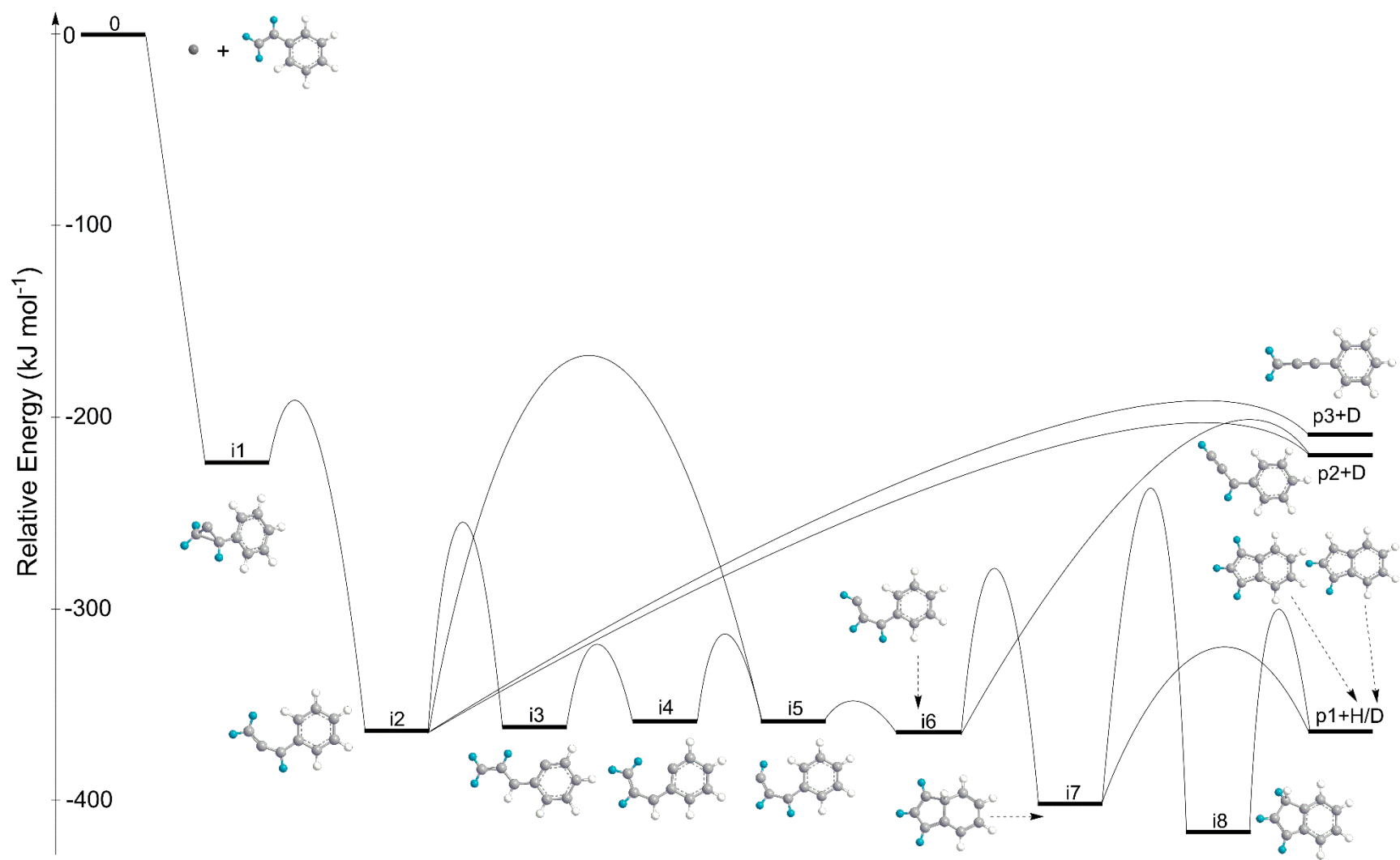


Fig. S4. PES of the reaction of atomic carbon (C) with D3-styrene.

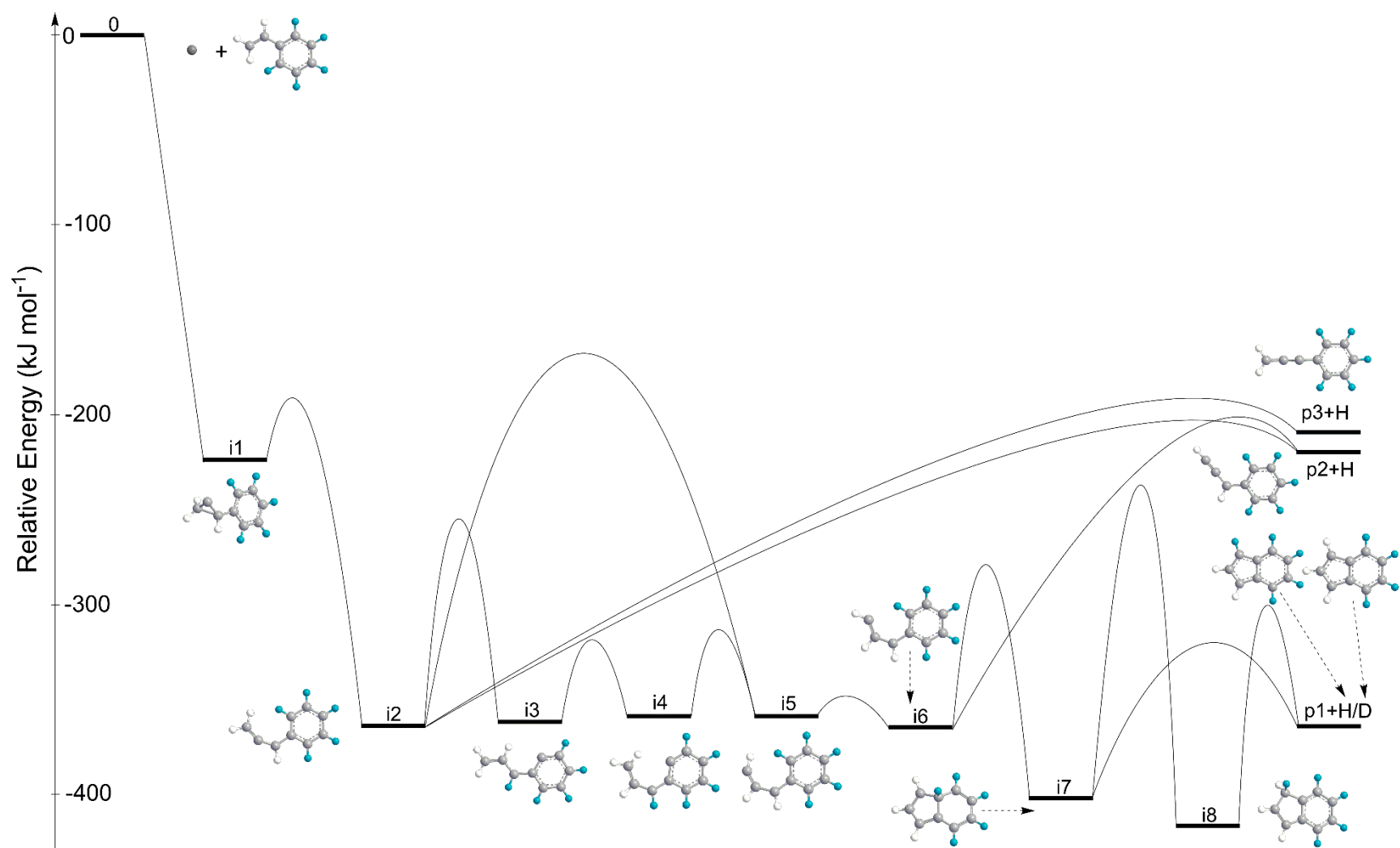


Fig. S5. PES of the reaction of atomic carbon (C) with D5-styrene.

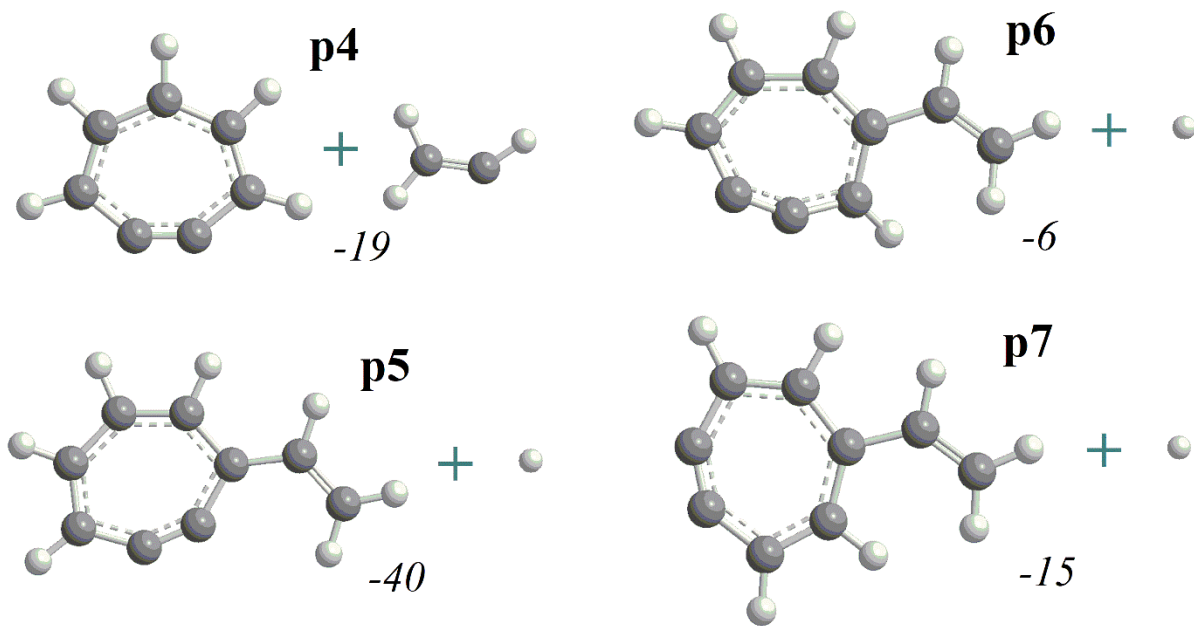


Fig. S6. Alternative reaction products originating from atomic carbon (C) addition to the benzene ring. Overall reaction energies are given in kJmol^{-1} .

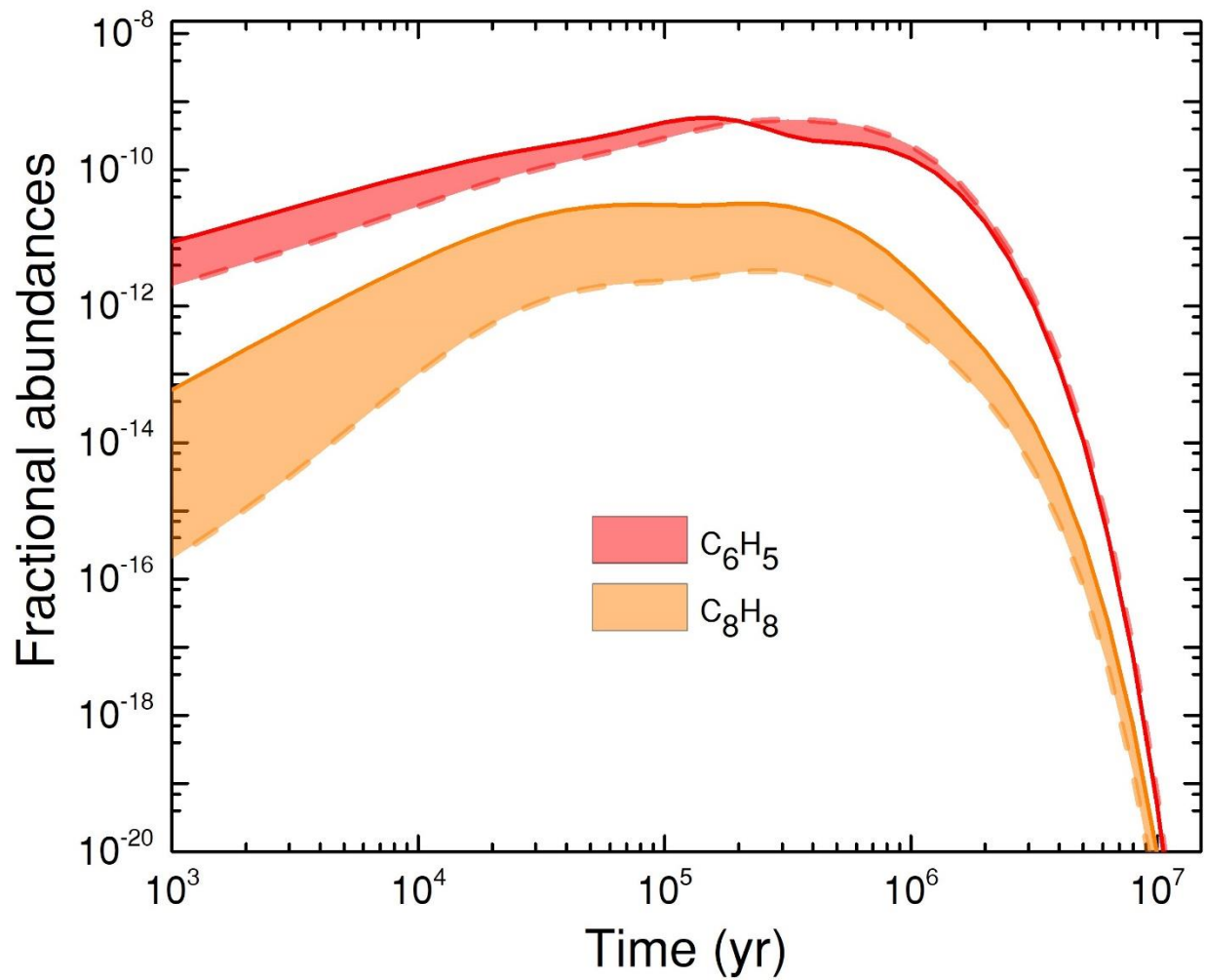


Fig. S7. Results of the astrochemical modeling of the fractional abundances of the gas-phase phenyl (C_6H_5 , red) and styrene (C_8H_8 , orange) versus time in TMC-1.

Table S1. Peak velocities (v_p) and speed ratios (S) of the carbon (C ; 3P), and styrene (C_8H_8 ; X^1A') reactants along with the corresponding collision energy (E_C) and center-of-mass angle (θ_{CM}).

Beam	v_p ($m\ s^{-1}$)	S	E_c ($kJ\ mol^{-1}$)	θ_{CM} (deg)
C	2534 ± 61	2.2 ± 0.3		
C_8H_8	389 ± 6	28.0 ± 0.4	35.4 ± 1.4	52.8 ± 0.6
$C_8H_5D_3$	386 ± 5	28.0 ± 0.4	35.5 ± 1.4	53.4 ± 0.6
$C_8H_3D_5$	385 ± 5	28.2 ± 0.5	35.5 ± 1.4	53.8 ± 0.6

Table S2. Statistical branching ratios (%) for the reaction of the atomic carbon with styrene. **p1**, **p2**, and **p3** denote 1-indenyl, 1-phenylpropargyl, and 3-phenylpropargyl, respectively.

E_C ($kJ\ mol^{-1}$)	i7→p1+H	i8→p1+H	i2→p2+H	i6→p2+H	i2→p3+H
35.4	54.7%	0.2%	29.5%	12.1%	3.5%

Table S3. Bimolecular reactions and photodissociation processes newly incorporated into the astrochemical model (Phys. Chem. Chem. Phys., 24, 25077-25087 (2022) (53)).

Reactant 1	Reactant 2	Products	α	β	γ	No.
CH ₂ CHCHCH ₂	CH ₃ CC	C ₇ H ₈ +H	4.00E-10	0	0	R1
C ₇ H ₈	CH	C ₈ H ₈ +H	2.00E-10	0	0	R2
C ₈ H ₈	CH	C ₉ H ₈ +H	4.00E-10	0	0	R3
C ₈ H ₈	C	C ₉ H ₇ +H	1.00E-10	0	0	R4
C ₉ H ₈	hν	C ₉ H ₇ +H	3.00E-09	0	3.1	R5
C ₆ H ₅	CH ₂ CCH	C ₉ H ₇ +H	4.00E-10	0	0	R6
C ₉ H ₈	CH	C ₁₀ H ₈ +H	2.00E-10	0	0	R7
C ₉ H ₈	C	C ₁₀ H ₇ +H	2.00E-10	0	0	R8
C ₉ H ₈	C	C ₁₀ H ₇ +H	2.00E-10	0	0	R9
C ₉ H ₇	CH ₂	C ₁₀ H ₈ +H	1.00E-11	0	0	R10
CH ₃ CCH	hν	CH ₃ CC+H	1.00E-09	0	3.1	R11
CH ₂ CHCHCH ₂	C ₄ H ₃	C ₈ H ₈ +H	4.00E-10	0	0	R12
C ₅ H ₆	C ₄ H ₃	C ₉ H ₈ +H	4.00E-10	0	0	R13
C ₃ H ₅	C ₆ H ₄	C ₉ H ₈ +H	4.00E-10	0	0	R14
CH	C ₂ H ₅	C ₃ H ₅ +H	4.00E-10	0	0	R15
CH ₃	C ₂ H ₃	C ₃ H ₅ +H	4.00E-10	0	0	R16
CH ₃ CHCH ₂	hν	C ₃ H ₅ +H	3.00E-09	0	3.1	R17
CH ₃ CH ₃	hν	C ₂ H ₅ +H	3.00E-09	0	3.1	R18
CH	CH ₃	C ₂ H ₃ +H	4.00E-10	0	0	R19
CH ₂	CH ₂	C ₂ H ₃ +H	4.00E-10	0	0	R20
C ₂ H ₄	hν	C ₂ H ₃ +H	3.00E-09	0	3.1	R21
C ₂ H	CH ₂ CHCCH	C ₆ H ₄ +H	4.00E-10	0	0	R22
CH ₂ CCH	C ₃ H ₂	C ₆ H ₄ +H	4.00E-10	0	0	R23
C ₂ H	C ₅ H ₈	C ₇ H ₈ +H	4.00E-10	0	0	R24
CH ₂ CCH ₂	C ₄ H ₅	C ₇ H ₈ +H	4.00E-10	0	0	R25
CH	C ₆ H ₈	C ₇ H ₈ +H	4.00E-10	0	0	R26
C ₂ H	C ₆ H ₈	C ₈ H ₈ +H	4.00E-10	0	0	R27
CH ₂ CHCCH	C ₄ H ₅	C ₈ H ₈ +H	4.00E-10	0	0	R28
C	CH ₃ CHCH ₂	C ₄ H ₅ +H	4.00E-10	0	0	R29
CH	C ₃ H ₅	C ₄ H ₅ +H	4.00E-10	0	0	R30
CH ₃	CH ₂ CCH	C ₄ H ₅ +H	4.00E-10	0	0	R31
C ₂ H	C ₂ H ₅	C ₄ H ₅ +H	4.00E-10	0	0	R32
C ₂ H ₃	C ₂ H ₃	C ₄ H ₅ +H	4.00E-10	0	0	R33
CH ₂ CHCHCH ₂	hν	C ₄ H ₅ +H	3.00E-09	0	3.1	R34
CH	C ₅ H ₈	C ₆ H ₈ +H	4.00E-10	0	0	R35
C ₂ H	C ₄ H ₈	C ₆ H ₈ +H	4.00E-10	0	0	R36
CH	C ₄ H ₈	C ₅ H ₈ +H	4.00E-10	0	0	R37
CH	C ₃ H ₈	C ₄ H ₈ +H	4.00E-10	0	0	R38
CH ₂ CHCHCH ₂	hν	CCCH ₂ CH ₃ +H	3.00E-09	0	3.1	R39
C ₄ H ₈	hν	C ₃ H ₇ +CH	1.00E-10	0	3.1	R40
C ₄ H ₅	hν	CH ₂ CHCCH+H	1.00E-10	0	3.1	R41

Table S4. Cartesian coordinates and frequencies (cm^{-1}) of reactants, intermediates, transition states, and products of the reaction of the atomic carbon with styrene.

Styrene

Geometry

6	0	0.514046	-0.220422	-0.002888
6	0	-0.406082	-1.279246	0.000138
6	0	-1.778225	-1.044039	0.002937
6	0	-2.261384	0.261196	0.002283
6	0	-1.359664	1.326960	-0.001276
6	0	0.008594	1.090363	-0.003925
6	0	1.953290	-0.528216	-0.004599
6	0	2.972003	0.334803	0.006259
1	0	-0.035896	-2.299492	0.000677
1	0	-2.468403	-1.880365	0.005433
1	0	-3.328938	0.449713	0.004174
1	0	-1.727932	2.346982	-0.002467
1	0	0.691241	1.932066	-0.007837
1	0	2.185844	-1.590967	-0.015687
1	0	2.831819	1.409900	0.018921
1	0	3.996802	-0.016229	0.003211

Frequencies

35.3757	205.2452	235.4052
411.9531	446.3442	448.8429
561.4898	635.0096	655.4358
710.5811	787.4429	798.7095
849.8200	927.6641	930.4721
976.3294	998.8183	1014.9399
1030.0462	1040.1559	1056.1697
1111.8838	1182.6896	1205.3639
1226.7313	1318.0793	1345.5572
1362.6204	1452.0525	1483.2868
1528.6315	1618.1117	1644.4888
1691.0547	3128.5909	3142.8072
3157.0921	3163.5676	3173.4637
3182.0512	3190.6412	3221.9594

T1 diagnostic: 0.01113239

ii

Geometry

6	0	-0.215485	-0.230976	0.192006
6	0	0.694515	-1.290061	0.065255
6	0	2.053346	-1.044749	-0.105171
6	0	2.526628	0.265293	-0.149612
6	0	1.631936	1.327484	-0.014888
6	0	0.274988	1.083336	0.160217
6	0	-1.660011	-0.516439	0.357309
6	0	-2.726099	0.091491	-0.759288
1	0	0.329530	-2.311652	0.097842
1	0	2.743374	-1.875562	-0.201844
1	0	3.585475	0.458012	-0.279782

1	0	1.996518	2.348551	-0.034540
1	0	-0.417573	1.907386	0.292469
1	0	-1.877977	-1.558170	0.601520
1	0	-2.261837	0.706301	-1.531365
1	0	-3.457508	-0.625746	-1.135878
6	0	-2.686485	0.473101	0.619434

Frequencies

65.7728	134.8951	205.8367
305.0955	413.6343	415.2449
518.2696	563.6138	620.5616
634.2629	709.3462	770.1980
777.4979	855.1419	887.4634
926.4720	934.6018	981.9999
995.0157	1003.6152	1015.4714
1029.9887	1042.7142	1051.3944
1103.5218	1181.8843	1197.0390
1212.9492	1236.8149	1315.0046
1349.7164	1378.5954	1462.2272
1487.8391	1521.6940	1618.2077
1638.0741	3040.3478	3061.1188
3110.8982	3157.0384	3163.5863
3172.4920	3180.0452	3190.1911

T1 diagnostic: 0.01717722

i2

Geometry

6	0	0.079961	-0.451806	-0.000057
6	0	-1.055674	-1.294362	0.000033
6	0	-2.339105	-0.769675	0.000107
6	0	-2.532440	0.613040	0.000055
6	0	-1.423887	1.463214	-0.000066
6	0	-0.137901	0.944682	-0.000123
6	0	1.395029	-1.049434	-0.000152
6	0	3.348497	0.700222	0.000114
6	0	2.624236	-0.423340	0.000076
1	0	-0.910454	-2.369584	0.000068
1	0	-3.193843	-1.436930	0.000206
1	0	-3.535239	1.024282	0.000090
1	0	-1.568051	2.537993	-0.000128
1	0	0.708470	1.618636	-0.000226
1	0	1.406176	-2.138904	-0.000354
1	0	2.905605	1.698604	0.000431
1	0	4.435035	0.670649	-0.000015

Frequencies

49.3026	148.6245	182.5179
269.0895	379.1257	410.8449
436.3462	470.7691	547.1465
616.4498	630.3712	693.2908
767.9936	792.8284	811.7296
812.9016	837.0860	912.7649
972.3835	985.7690	996.3692
1004.4258	1038.6132	1052.6698
1109.5126	1180.2917	1188.3043

1229.7448	1310.5145	1349.8284
1385.9547	1428.2883	1485.2098
1494.5200	1537.5851	1598.3041
1626.3663	3048.2449	3102.3288
3143.8481	3159.7422	3167.5426
3176.7102	3189.7736	3206.8961

T1 diagnostic: 0.01650379

i7

Geometry

6	0	0.261972	0.764914	0.212259
6	0	-0.903809	1.442584	0.058714
6	0	-2.145806	0.709483	-0.052096
6	0	-2.126835	-0.679204	-0.213335
6	0	-0.961239	-1.412918	-0.070527
6	0	0.268134	-0.736537	0.455712
6	0	1.632221	1.161627	-0.041292
6	0	1.633163	-1.136226	-0.060041
6	0	2.396701	0.011923	-0.251064
1	0	-0.905842	2.515578	-0.104793
1	0	-3.079232	1.252555	-0.136174
1	0	-3.048912	-1.191675	-0.468490
1	0	-0.957295	-2.488491	-0.207197
1	0	0.280165	-0.879761	1.562689
1	0	1.967503	2.180254	-0.182884
1	0	1.976976	-2.157566	-0.150414
1	0	3.439619	0.015223	-0.542720

Frequencies

145.1358	187.7739	356.7823
376.0554	495.2877	518.5817
527.7002	553.3295	623.2422
630.1519	694.0262	720.8333
746.9534	807.4062	824.3680
864.6289	871.0273	935.6624
943.0859	984.8345	1018.4619
1024.6016	1070.9140	1088.5575
1119.2289	1156.5125	1176.5979
1210.8923	1253.4508	1283.5656
1337.0215	1385.3330	1392.9782
1441.8452	1461.0773	1496.7520
1631.0774	2754.5792	3154.8291
3158.7143	3176.0994	3189.0867
3191.2289	3208.5503	3218.9773

T1 diagnostic: 0.01636376

i5

Geometry

6	0	0.149199	-0.413517	-0.067465
6	0	-0.940725	-1.308075	0.053747
6	0	-2.248373	-0.852106	0.118501
6	0	-2.518828	0.515793	0.051788
6	0	-1.462027	1.416699	-0.089511

6	0	-0.151119	0.965391	-0.149281
6	0	1.479808	-0.961978	-0.121530
6	0	3.061680	0.961713	0.232019
6	0	2.736595	-0.318760	-0.037870
1	0	-0.739343	-2.372932	0.106559
1	0	-3.061703	-1.562142	0.219257
1	0	-3.540371	0.874825	0.100242
1	0	-1.664684	2.479655	-0.161369
1	0	0.647586	1.679346	-0.295677
1	0	1.525707	-2.041890	-0.227683
1	0	2.608805	1.899806	0.507268
1	0	3.586738	-0.987627	-0.190992

Frequencies

47.8964	153.9771	178.8663
308.8588	321.1828	412.4315
468.5492	503.1410	624.1491
628.6939	652.3997	696.9125
719.5674	784.9770	801.6812
839.6482	874.8233	908.0388
920.6680	975.1614	996.8422
1006.4401	1044.3693	1092.2600
1114.3845	1180.6976	1196.8322
1242.3448	1272.5577	1323.7604
1350.3906	1394.9184	1468.7871
1496.7357	1520.4624	1599.1951
1622.5389	3069.9144	3148.9559
3159.2795	3166.3744	3176.2580
3189.3667	3208.3905	3259.9751

T1 diagnostic: 0.01446614

i4

Geometry

6	0	0.122090	-0.454006	-0.000010
6	0	-1.024918	-1.300578	0.000020
6	0	-2.310485	-0.782309	0.000028
6	0	-2.528808	0.599663	0.000000
6	0	-1.429403	1.472859	-0.000028
6	0	-0.182785	0.907992	-0.000023
6	0	1.437153	-1.022996	-0.000020
6	0	2.916206	0.988992	0.000050
6	0	2.681274	-0.356019	-0.000033
1	0	-0.872610	-2.375739	0.000042
1	0	-3.157772	-1.458611	0.000056
1	0	-3.537533	0.997815	0.000002
1	0	-1.572908	2.548076	-0.000054
1	0	1.470326	-2.108084	-0.000045
1	0	3.929258	1.372556	0.000107
1	0	3.550552	-1.009946	-0.000087
1	0	2.108749	1.712336	0.000074

Frequencies

74.2780	149.7396	155.5280
308.3819	315.3196	419.9307
465.1608	514.0335	582.5593

621.3501	661.9885	687.8091
735.8383	790.5770	821.3762
853.9287	854.8657	934.0741
976.7554	977.9408	995.8364
1014.5630	1041.1711	1114.8373
1131.2181	1171.5644	1212.4116
1265.2020	1272.6212	1327.4483
1407.8970	1441.1331	1458.6382
1468.3136	1546.6624	1558.4944
1606.5520	3127.7950	3131.2794
3152.0429	3159.9751	3161.6987
3173.2076	3186.9475	3225.6417

T1 diagnostic: 0.01649022

i8

Geometry

6	0	0.211416	0.766354	-0.000016
6	0	-1.080084	1.408472	-0.000086
6	0	-2.211035	0.633773	-0.000017
6	0	-2.135561	-0.783048	0.000066
6	0	-0.881219	-1.435692	0.000027
6	0	0.270064	-0.693564	-0.000053
6	0	1.480021	1.283016	0.000099
6	0	1.723066	-1.145188	-0.000075
6	0	2.459774	0.168657	0.000113
1	0	-1.143985	2.490759	-0.000213
1	0	-3.187212	1.106693	-0.000032
1	0	-3.047672	-1.367513	0.000193
1	0	-0.842328	-2.520554	0.000061
1	0	1.742222	2.332213	0.000205
1	0	1.963081	-1.768467	-0.876639
1	0	1.963020	-1.768748	0.876297
1	0	3.534230	0.278944	-0.000221

Frequencies

84.6402	189.9057	214.3995
282.8862	387.4210	406.8425
494.9251	530.7006	576.9660
677.7698	699.4214	700.1590
759.5214	782.4508	821.5316
871.7001	884.4326	906.9716
953.7445	970.0242	983.0080
1011.1259	1089.4429	1123.2007
1136.2093	1156.6778	1196.9463
1263.8936	1303.5421	1317.8898
1352.3815	1417.6078	1426.4553
1475.4717	1528.4357	1569.9028
1598.7293	2929.4012	2935.8046
3156.7794	3162.5154	3179.3601
3191.0151	3207.6623	3226.6856

T1 diagnostic: 0.01322213

i3

Geometry

6	0	-0.044571	-0.250171	0.000001
6	0	0.943611	-1.276534	0.000010
6	0	2.297898	-0.977371	-0.000005
6	0	2.743617	0.348556	-0.000031
6	0	1.803999	1.394798	-0.000041
6	0	0.483131	1.045430	-0.000023
6	0	-1.439519	-0.557263	0.000016
6	0	-3.805760	0.095892	0.000040
6	0	-2.475769	0.396358	0.000023
1	0	0.615034	-2.311496	0.000031
1	0	3.021295	-1.784885	0.000004
1	0	3.804441	0.573164	-0.000044
1	0	2.125349	2.430897	-0.000061
1	0	-1.712217	-1.609289	0.000024
1	0	-4.560435	0.872118	0.000044
1	0	-4.152782	-0.932117	0.000049
1	0	-2.180498	1.443427	0.000014

Frequencies

96.5456	136.5154	158.2705
247.1154	358.2291	407.3711
420.1810	505.4915	607.9355
609.7634	627.8219	688.1822
735.0938	806.6296	840.7812
847.5708	862.2729	929.5248
974.8143	975.5786	993.0135
1011.9246	1034.4785	1110.8227
1168.2839	1187.3461	1214.5193
1260.4096	1295.9558	1324.8272
1371.8879	1428.0484	1459.2723
1481.4151	1536.0346	1556.4945
1605.8573	3130.8197	3136.6614
3146.7425	3152.8350	3160.6563
3172.9523	3187.0769	3229.3401

T1 diagnostic: 0.01655292

i6

Geometry

6	0	0.129187	-0.432149	-0.000144
6	0	-0.985594	-1.303275	-0.000216
6	0	-2.283065	-0.814569	-0.000038
6	0	-2.513807	0.562362	0.000143
6	0	-1.428528	1.441187	0.000080
6	0	-0.128318	0.957523	-0.000081
6	0	1.450634	-1.001333	0.000172
6	0	2.968919	0.979616	-0.000340
6	0	2.695360	-0.341816	0.000182
1	0	-0.813478	-2.374717	-0.000392
1	0	-3.119086	-1.505181	-0.000061
1	0	-3.527427	0.946544	0.000344
1	0	-1.600821	2.511892	0.000197
1	0	0.705815	1.650023	-0.000024
1	0	1.491712	-2.085904	0.000619
1	0	3.867477	1.578585	0.000277

1 0 3.567080 -1.006518 0.000491
Frequencies

69.4785	166.6716	169.1752
319.8317	343.4346	412.0422
472.4967	514.5661	569.5091
630.4218	654.0584	692.0060
725.5976	784.1013	812.4824
842.0113	877.2272	894.3287
919.3877	975.2656	997.1074
1005.8502	1043.8778	1103.4290
1116.5560	1179.9588	1194.7987
1241.6497	1257.9779	1326.5426
1351.4078	1410.0489	1469.2732
1499.2026	1521.1423	1598.9999
1622.3186	3022.2059	3155.2804
3157.7967	3160.8741	3169.8843
3177.2070	3189.7630	3235.3410

T1 diagnostic: 0.01412565

ts_i1_i2

Geometry

6	0	-0.165477	-0.263583	0.213034
6	0	0.773138	-1.300347	0.027021
6	0	2.117276	-1.015393	-0.164062
6	0	2.558833	0.309540	-0.182073
6	0	1.642332	1.347153	-0.001637
6	0	0.296360	1.069219	0.191992
6	0	-1.561157	-0.573325	0.435315
6	0	-3.059907	0.169184	-0.720820
6	0	-2.621356	0.390651	0.581663
1	0	0.432286	-2.330535	0.037601
1	0	2.825899	-1.824632	-0.301132
1	0	3.608907	0.530899	-0.334972
1	0	1.983049	2.376617	-0.008704
1	0	-0.416764	1.871595	0.343793
1	0	-1.816991	-1.628757	0.520810
1	0	-2.490055	0.529343	-1.578345
1	0	-4.006582	-0.323119	-0.961649

Frequencies

-581.5527	94.8382	109.4257
212.5191	271.1443	414.8787
423.0137	502.8604	566.0433
630.8641	697.4933	702.8537
752.1472	784.7732	815.7788
850.3651	900.5939	925.6204
963.5585	980.5651	1001.6721
1008.1190	1042.8431	1078.8562
1106.8700	1167.6840	1180.4254
1204.0936	1229.7884	1316.7723
1349.5826	1371.5295	1457.0233
1486.1929	1513.8086	1603.7743
1626.2285	3031.0657	3099.4986
3108.6036	3158.0846	3164.7875

3174.1203 3181.5120 3190.6853
T1 diagnostic: 0.01895232

ts_i6_i7

Geometry

6	0	0.248729	0.626447	0.374502
6	0	-0.808622	1.399009	-0.054632
6	0	-2.053480	0.813996	-0.333488
6	0	-2.220461	-0.559880	-0.209205
6	0	-1.185273	-1.354259	0.266219
6	0	0.072609	-0.787378	0.567530
6	0	1.652580	1.039439	0.309176
1	0	-0.656549	2.458078	-0.235485
1	0	-2.875599	1.434225	-0.671158
1	0	-3.180227	-1.009487	-0.438713
1	0	-1.352921	-2.408871	0.453424
1	0	0.672809	-1.280741	1.326686
1	0	1.990889	2.046375	0.516195
6	0	1.814639	-1.137550	-0.547790
6	0	2.443408	0.053933	-0.267748
1	0	2.124721	-2.027570	-1.078684
1	0	3.492108	0.225450	-0.499648

Frequencies

-652.7780	141.3013	198.1422
309.6842	405.2001	473.3952
503.5583	524.2928	546.4956
611.4606	673.7952	698.2460
737.2882	765.8598	802.6825
855.9776	888.4415	927.0829
934.3187	957.1485	996.2264
1018.6167	1050.8038	1078.0809
1099.8241	1160.4733	1181.1220
1194.6327	1220.8014	1320.4839
1335.5541	1385.1445	1427.1422
1473.8261	1522.6490	1596.6262
1627.0917	3157.6537	3159.7734
3187.6650	3194.4438	3206.6199
3219.2829	3230.3459	3240.5394

T1 diagnostic: 0.02348279

ts_i2_i5

Geometry

6	0	0.085909	-0.454691	-0.000236
6	0	-1.047784	-1.300861	0.000055
6	0	-2.331740	-0.777769	0.000254
6	0	-2.526834	0.605011	0.000153
6	0	-1.419977	1.458348	-0.000127
6	0	-0.133301	0.942892	-0.000328
6	0	1.402175	-1.035732	-0.000260
6	0	3.332805	0.773973	0.000487
6	0	2.608744	-0.331215	0.000017
1	0	-0.900367	-2.375831	0.000141

1	0	-3.185948	-1.445732	0.000486
1	0	-3.530486	1.014233	0.000276
1	0	-1.567285	2.532694	-0.000199
1	0	0.715874	1.614472	-0.000521
1	0	1.454486	-2.120037	-0.000468
1	0	3.275595	1.865386	0.000324
1	0	3.918142	-0.364933	-0.000127

Frequencies

-2146.3606	65.5710	134.8348
163.0597	217.6736	303.4082
362.7427	409.9671	453.7721
514.1097	607.8230	628.5143
650.2154	693.9841	758.9835
797.1944	827.5133	839.5200
863.7053	915.5620	974.9695
997.0620	1003.5239	1036.8961
1052.6660	1109.7588	1179.8140
1188.1275	1232.9044	1313.1050
1349.9081	1393.4366	1484.5033
1506.2804	1596.1422	1602.2167
1658.5708	2321.5348	3021.1226
3151.1542	3159.6437	3167.1784
3176.3172	3188.9065	3199.2458

T1 diagnostic: 0.01528249

ts_i4_i5

Geometry

6	0	0.153664	-0.560317	-0.000004
6	0	-1.023169	-1.343802	0.000004
6	0	-2.270888	-0.734374	0.000031
6	0	-2.386917	0.659467	0.000013
6	0	-1.235669	1.459775	-0.000032
6	0	-0.008463	0.834601	-0.000014
6	0	1.477686	-1.116749	-0.000037
6	0	2.517737	1.069574	0.000079
6	0	2.620722	-0.288440	-0.000003
1	0	-0.943474	-2.426424	-0.000013
1	0	-3.166160	-1.346029	0.000037
1	0	-3.367511	1.122981	0.000018
1	0	-1.319481	2.541294	-0.000105
1	0	1.229931	1.375018	0.000024
1	0	1.593833	-2.194470	-0.000088
1	0	3.304168	1.813823	-0.000131
1	0	3.600476	-0.764607	0.000040

Frequencies

-1643.3108	133.4667	196.3996
301.8145	394.0122	432.5343
461.6447	510.5185	523.9844
612.7951	646.3093	698.4582
724.6605	740.7562	780.0338
840.8054	863.7523	915.6681
937.5568	965.8686	984.8435
985.0352	1007.5157	1039.0726

1100.6738	1131.0166	1173.5465
1220.5353	1251.3781	1272.9343
1326.9491	1372.5691	1453.1622
1458.4457	1485.5749	1574.6951
1595.4765	1647.4505	3108.0056
3154.5348	3161.1689	3172.1928
3180.6131	3184.9328	3198.0617

T1 diagnostic: 0.01488586

ts_i8_p1

Geometry

6	0	0.276386	0.679713	-0.044049
6	0	-0.881301	1.435331	-0.060280
6	0	-2.121831	0.780662	-0.029585
6	0	-2.211005	-0.625190	0.026719
6	0	-1.067616	-1.401060	0.048900
6	0	0.198139	-0.763212	0.007022
6	0	1.694686	1.056218	-0.026037
6	0	1.498229	-1.266246	-0.014130
6	0	2.419735	-0.120211	-0.111756
1	0	-0.840261	2.518850	-0.085806
1	0	-3.032924	1.368346	-0.042389
1	0	-3.187134	-1.095097	0.052930
1	0	-1.132547	-2.483021	0.090171
1	0	2.067606	2.035952	-0.289083
1	0	1.792907	-2.306007	0.014591
1	0	2.004516	1.505162	1.660709
1	0	3.495306	-0.200203	-0.181940

Frequencies

-1159.4112	185.7193	215.4160
354.0884	386.7747	407.4167
485.0239	521.8739	539.7448
579.8552	604.5356	704.9075
746.3123	755.4944	765.1637
804.2945	842.6184	870.1122
883.1005	948.3204	974.4017
981.4236	1008.7610	1020.3673
1075.0173	1126.4261	1147.9728
1182.3401	1204.4145	1283.3888
1329.8323	1359.2931	1378.6251
1418.3699	1486.6997	1512.1202
1578.0888	1598.1820	3163.4137
3169.2725	3179.5557	3191.4329
3203.7999	3215.1886	3227.9525

T1 diagnostic: 0.01952452

ts_i2_i3

Geometry

6	0	-0.007534	-0.567598	-0.000206
6	0	1.165234	-1.346013	-0.000007
6	0	2.400513	-0.703947	0.000142
6	0	2.494178	0.692003	0.000131

6	0	1.331560	1.487481	-0.000066
6	0	0.124322	0.837577	-0.000385
6	0	-1.384383	-0.959307	-0.000082
6	0	-3.562606	0.385985	0.000099
6	0	-2.240150	0.160686	0.000230
1	0	1.107477	-2.429522	0.000151
1	0	3.309283	-1.295538	0.000346
1	0	3.469402	1.166671	0.000233
1	0	1.405800	2.569525	-0.000138
1	0	-1.239492	1.103850	0.000295
1	0	-1.729130	-1.988005	-0.000186
1	0	-3.973696	1.388887	0.000642
1	0	-4.276444	-0.437069	-0.000479

Frequencies

-1941.4222	108.2992	210.1737
235.0883	313.1399	411.7391
411.9203	447.9478	513.8548
611.1361	621.9781	651.5800
714.0703	734.0564	777.9758
830.9198	862.5507	862.7435
934.6131	952.0085	982.3476
982.7006	1026.4015	1086.6993
1115.2593	1141.3428	1172.8284
1192.8046	1259.2726	1312.7557
1346.0567	1409.9384	1447.8757
1472.7368	1541.4582	1587.2649
1599.1936	1738.8772	3090.2248
3157.1574	3163.8907	3168.6149
3173.6404	3185.1752	3193.2975

T1 diagnostic: 0.01660469

ts_i7_p1

Geometry

6	0	0.262542	0.735382	0.067446
6	0	-0.919868	1.434791	0.010349
6	0	-2.139516	0.718354	-0.034489
6	0	-2.154943	-0.673783	-0.097981
6	0	-0.965469	-1.404300	-0.061787
6	0	0.252355	-0.714925	0.146370
6	0	1.656617	1.146077	-0.019429
6	0	1.624348	-1.139603	-0.071155
6	0	2.442437	0.007975	-0.120565
1	0	-0.927412	2.518802	-0.030631
1	0	-3.074850	1.265358	-0.065153
1	0	-3.101256	-1.194117	-0.190687
1	0	-0.978572	-2.486685	-0.123496
1	0	0.248928	-0.763330	1.879285
1	0	2.004761	2.169655	-0.038091
1	0	1.958468	-2.166549	-0.123361
1	0	3.518913	-0.002942	-0.220420

Frequencies

-912.9403	200.9617	228.4893
375.8982	409.8936	482.7130

531.8597	539.1039	553.0510
576.8906	611.4139	709.8034
740.1579	746.6976	762.9098
804.0419	863.3329	866.4852
889.0109	914.2198	936.2437
973.1462	1026.4134	1028.6548
1086.0760	1097.0003	1173.1040
1182.3811	1200.1137	1233.2341
1329.4644	1360.5335	1381.1474
1448.2289	1477.7178	1487.9608
1575.6901	1619.4035	3163.5950
3170.1921	3180.1983	3191.7338
3204.6381	3215.2872	3228.4796

T1 diagnostic: 0.01697420

ts_i3_i4

Geometry

6	0	0.024002	-0.019771	0.286166
6	0	-0.706343	1.176246	0.129017
6	0	-2.077405	1.153799	-0.121323
6	0	-2.765546	-0.054544	-0.221363
6	0	-2.072349	-1.262759	-0.069396
6	0	-0.723798	-1.175928	0.176263
1	0	-0.180967	2.122902	0.204546
1	0	-2.612240	2.089293	-0.240354
1	0	-3.832630	-0.064447	-0.416538
1	0	-2.584509	-2.215801	-0.144304
6	0	1.481903	-0.016157	0.561947
6	0	3.814900	-0.045094	-0.201184
6	0	2.452979	-0.050170	-0.429163
1	0	1.793543	0.007457	1.604141
1	0	4.523251	-0.075018	-1.018891
1	0	4.215144	-0.013587	0.806279
1	0	2.108342	-0.084532	-1.460662

Frequencies

-142.8904	103.9905	118.7579
290.8994	353.8595	370.7908
414.4352	503.9607	539.2226
611.7174	630.3211	705.1225
734.9757	744.5460	805.4009
826.7593	861.5850	945.2386
986.2886	986.8540	994.6225
999.7625	1044.0739	1116.2750
1173.1233	1197.9514	1212.7989
1238.4482	1279.8968	1311.0995
1329.7365	1429.8099	1468.0016
1490.1737	1516.0199	1565.8905
1630.0137	3124.2285	3135.8961
3139.6331	3156.4845	3163.0105
3173.5957	3186.1626	3235.5921

T1 diagnostic: 0.01368756

ts_i5_i6

Geometry

6	0	0.137180	-0.429203	-0.000069
6	0	-0.974555	-1.305679	0.000076
6	0	-2.274641	-0.824721	0.000145
6	0	-2.513868	0.550878	0.000053
6	0	-1.433188	1.435178	-0.000110
6	0	-0.130075	0.959346	-0.000169
6	0	1.457831	-0.996897	-0.000151
6	0	3.020338	0.951629	0.000247
6	0	2.719031	-0.350417	-0.000041
1	0	-0.796711	-2.376116	0.000143
1	0	-3.106407	-1.520462	0.000270
1	0	-3.529623	0.929345	0.000097
1	0	-1.611613	2.504956	-0.000204
1	0	0.696827	1.657732	-0.000318
1	0	1.496834	-2.082130	-0.000311
1	0	3.236221	1.994441	0.000658
1	0	3.566151	-1.048452	-0.000215

Frequencies

-702.3492	59.5328	162.0125
173.9979	302.6632	321.9631
346.9396	412.2877	481.5091
511.2078	630.4867	693.4525
698.2440	713.9566	782.4394
822.7356	838.0059	877.9321
916.3594	973.7352	996.2504
1005.3940	1043.0564	1086.9304
1113.4810	1179.8969	1193.4413
1242.6359	1282.7657	1322.2344
1348.9427	1388.5183	1467.7394
1497.8748	1519.6219	1597.8023
1620.9544	2993.4772	3151.5813
3158.6563	3164.9262	3175.2106
3187.1224	3194.3164	3422.4598

T1 diagnostic: 0.01556471

ts_i2_p2

Geometry

6	0	0.039618	-0.377165	0.000010
6	0	-1.028562	-1.297628	-0.000013
6	0	-2.340537	-0.860579	-0.000023
6	0	-2.625107	0.503151	-0.000013
6	0	-1.581579	1.427352	0.000005
6	0	-0.267028	0.999555	0.000018
6	0	1.387334	-0.855172	0.000028
6	0	3.574780	0.559308	-0.000054
6	0	2.510722	-0.040504	0.000085
1	0	-0.810434	-2.360524	-0.000022
1	0	-3.148328	-1.583428	-0.000038
1	0	-3.653756	0.844629	-0.000018
1	0	-1.799806	2.489296	0.000014

1	0	0.543029	1.720530	0.000035
1	0	1.555923	-1.928476	0.000014
1	0	4.345282	1.294338	-0.000157
1	0	4.950250	-0.826273	-0.000087

Frequencies

-795.2583	86.2594	114.1463
158.7428	226.8983	279.2671
374.6401	405.9963	442.3546
485.2813	487.9485	572.9333
631.0782	646.6487	688.0286
699.7908	783.4408	830.8542
843.1734	850.0495	928.4369
996.1072	1009.7730	1012.2548
1052.0452	1073.4749	1123.0281
1183.2653	1194.4512	1236.8471
1327.2929	1356.7736	1411.3405
1499.3045	1522.4456	1626.6708
1641.2131	2039.4535	3177.6053
3189.8690	3194.9654	3205.9768
3215.1283	3223.1168	3454.0260

T1 diagnostic: 0.01607936

ts_i2_p3

Geometry

6	0	0.015604	0.137963	-0.000005
6	0	-0.841264	1.250178	-0.000002
6	0	-2.214998	1.075550	0.000002
6	0	-2.762798	-0.203135	0.000005
6	0	-1.924248	-1.314660	0.000001
6	0	-0.550335	-1.151845	-0.000004
6	0	1.431024	0.257602	-0.000006
6	0	3.976825	-0.198902	0.000006
6	0	2.634182	-0.055435	-0.000003
1	0	-0.409474	2.243978	-0.000005
1	0	-2.864357	1.943462	0.000005
1	0	-3.838706	-0.334465	0.000009
1	0	-2.346368	-2.313023	0.000004
1	0	0.107171	-2.012989	-0.000007
1	0	1.712376	2.192880	0.000006
1	0	4.436769	-1.179388	0.000007
1	0	4.618642	0.675651	0.000016

Frequencies

-768.1047	70.2772	118.7338
129.9462	256.7985	322.3637
380.0717	413.9169	417.6851
443.4309	530.8136	546.0859
581.3415	640.9859	701.7507
716.0843	744.8888	773.6741
861.2334	940.6835	1000.6078
1016.5291	1016.8346	1017.3617
1051.6122	1076.9787	1114.5988
1187.4819	1205.1723	1312.6862
1351.6816	1353.4270	1466.6764

1485.8231	1534.1960	1632.0335
1651.8794	1966.0419	3152.1747
3193.6339	3202.6913	3212.0881
3218.8088	3225.5443	3252.6662

T1 diagnostic: 0.01726148

ts_i6_p2

Geometry

6	0	0.083330	-0.408053	-0.000021
6	0	-1.011028	-1.297170	-0.000006
6	0	-2.310734	-0.824349	0.000017
6	0	-2.557174	0.546415	0.000020
6	0	-1.487709	1.439647	-0.000003
6	0	-0.184971	0.975276	-0.000022
6	0	1.414657	-0.940951	-0.000030
6	0	3.335776	0.804309	0.000012
6	0	2.563931	-0.149512	0.000002
1	0	-0.822826	-2.365827	-0.000011
1	0	-3.137819	-1.525147	0.000033
1	0	-3.575656	0.917236	0.000044
1	0	-1.675642	2.507415	0.000000
1	0	0.642729	1.674888	-0.000038
1	0	1.534313	-2.017480	-0.000053
1	0	4.119664	1.523987	0.000037
1	0	3.838763	-1.588751	0.000172

Frequencies

-805.9905	34.2593	91.0674
155.1476	215.0976	346.1044
407.5924	445.3632	454.7184
477.5577	516.3320	550.8779
631.0907	647.4862	675.3102
683.2010	700.7937	784.5730
847.7230	850.5907	929.7228
996.0294	1010.7654	1012.3520
1053.5583	1074.7825	1127.7163
1183.9336	1201.6213	1242.5904
1326.9339	1360.2828	1410.1482
1499.2833	1525.0125	1628.6458
1642.6350	1966.1233	3190.7902
3197.4816	3208.0409	3210.0129
3218.4974	3225.1459	3462.7859

T1 diagnostic: 0.01658002

ts_i7_i8

Geometry

6	0	0.276139	0.736849	0.035786
6	0	-0.970130	1.446883	0.021417
6	0	-2.212089	0.665527	0.011959
6	0	-2.209230	-0.679603	-0.038768
6	0	-0.955955	-1.437689	-0.067677
6	0	0.264691	-0.682570	0.036287
6	0	1.606915	1.163744	-0.038264

6	0	1.683485	-1.111871	-0.000354
6	0	2.471480	0.052880	-0.073045
1	0	-1.000479	2.525383	-0.058467
1	0	-3.154702	1.200338	0.044184
1	0	-3.143758	-1.228075	-0.049205
1	0	-0.952233	-2.518327	-0.115107
1	0	1.045840	-1.041668	1.106690
1	0	1.925360	2.198351	-0.038773
1	0	1.997920	-2.137668	-0.136177
1	0	3.550216	0.076764	-0.077184

Frequencies

-1407.4293	137.6655	227.0030
288.1386	353.7495	385.0893
482.1253	505.3613	554.0275
562.1230	574.0399	697.8793
703.1941	718.7788	739.7238
841.5144	870.8032	883.2380
886.0799	912.6717	972.9323
996.1213	1019.3525	1061.4826
1137.2967	1170.7104	1195.8152
1217.7138	1233.3890	1284.8782
1337.3094	1376.2267	1405.3455
1434.8826	1485.0225	1529.2285
1674.2069	2031.5851	3195.3099
3214.4560	3222.9470	3227.4572
3233.5684	3242.8043	3268.2488

T1 diagnostic: 0.01905981

p1

Geometry

6	0	0.257873	-0.714080	-0.000110
6	0	-0.939058	-1.414883	0.000049
6	0	-2.146221	-0.695897	0.000102
6	0	-2.146184	0.695909	-0.000001
6	0	-0.939011	1.414919	-0.000079
6	0	0.257935	0.714150	-0.000059
6	0	1.645548	-1.140163	-0.000055
6	0	1.645679	1.140155	0.000001
6	0	2.457866	-0.000090	0.000064
1	0	-0.950850	-2.499821	0.000126
1	0	-3.088133	-1.232569	0.000318
1	0	-3.088060	1.232616	-0.000069
1	0	-0.950827	2.499840	-0.000252
1	0	1.986232	-2.166928	-0.000603
1	0	1.986480	2.166889	0.000477
1	0	3.538595	-0.000146	0.000535

Frequencies

200.0528	239.9979	391.4594
414.5034	534.6487	549.2933
560.0659	579.2704	713.1263
744.0297	754.2839	759.9115
804.3334	864.6468	874.9597
887.8542	902.5452	943.3469

979.3343	1013.2690	1034.1562
1081.1749	1092.4737	1181.1158
1185.0015	1212.0588	1219.3442
1328.9910	1371.9104	1384.0846
1463.8448	1488.1757	1489.7934
1617.7960	1625.2661	3159.9608
3165.4495	3175.9723	3189.2296
3202.9853	3209.7156	3228.3663

T1 diagnostic: 0.01219578

p2

Geometry

6	0	-0.119436	-0.397975	0.000433
6	0	0.976568	-1.294374	-0.000011
6	0	2.280706	-0.826227	-0.000457
6	0	2.535831	0.547576	-0.000355
6	0	1.466664	1.448831	0.000185
6	0	0.159695	0.990342	0.000550
6	0	-1.455464	-0.911064	0.000600
6	0	-3.626337	0.524842	-0.001946
6	0	-2.607417	-0.137910	0.000487
1	0	0.783060	-2.361940	-0.000120
1	0	3.105453	-1.530148	-0.000913
1	0	3.556403	0.912477	-0.000706
1	0	1.660651	2.515738	0.000288
1	0	-0.666547	1.691484	0.000898
1	0	-1.583065	-1.989530	0.000801
1	0	-4.520811	1.097680	0.002829

Frequencies

86.7333	124.1656	216.9788
329.4198	399.2084	427.4717
435.0745	479.0376	517.6060
628.8102	639.6427	665.7100
685.8713	705.1291	781.8774
835.7387	842.0967	916.3963
978.0637	997.7302	1002.3911
1040.1334	1069.8818	1112.8485
1178.8338	1186.6285	1231.0718
1321.4268	1352.1999	1407.0372
1486.5987	1507.7258	1592.7200
1611.0557	2075.1448	3150.3199
3160.3426	3166.6934	3176.5620
3186.1827	3193.0092	3469.9095

T1 diagnostic: 0.01558819

p3

Geometry

6	0	0.051010	-0.000210	-0.000277
6	0	-0.672854	1.214997	-0.000136
6	0	-2.059558	1.208019	0.000111
6	0	-2.760471	0.000244	0.000232
6	0	-2.059915	-1.207736	0.000109

6	0	-0.673203	-1.215188	-0.000142
6	0	1.456659	-0.000220	-0.000373
6	0	4.043940	0.000246	0.000297
6	0	2.689997	-0.000394	-0.000143
1	0	-0.126697	2.150425	-0.000206
1	0	-2.600109	2.147878	0.000216
1	0	-3.844340	0.000401	0.000452
1	0	-2.600784	-2.147415	0.000230
1	0	-0.127391	-2.150817	-0.000220
1	0	4.603254	-0.927932	0.000768
1	0	4.602431	0.928917	0.000694

Frequencies

88.9565	93.8913	243.4949
256.3229	309.8435	411.0115
412.6777	437.6422	528.7189
528.8661	634.3281	697.0315
718.4978	731.0154	769.4110
845.0897	923.6210	979.6987
999.4894	1002.6316	1029.5927
1040.5866	1066.4686	1101.1063
1180.8958	1197.8811	1306.1961
1350.6396	1363.4252	1469.3010
1470.6176	1526.3478	1592.0378
1618.5540	2075.9997	3133.5882
3165.0775	3172.9476	3185.3678
3192.6501	3196.8183	3219.4767

T1 diagnostic: 0.01668443

p4

Geometry

6	0	-1.312408	0.834565	0.000299
6	0	0.000417	1.401924	-0.000244
6	0	1.312678	0.834256	-0.000302
6	0	1.710472	-0.489748	0.000141
6	0	0.608836	-1.384724	0.000585
6	0	-0.609539	-1.385075	-0.000698
6	0	-1.710605	-0.488993	0.000052
1	0	-2.113260	1.571765	0.000777
1	0	0.000502	2.486538	-0.000476
1	0	2.113918	1.571045	-0.000523
1	0	2.751009	-0.781861	0.000969
1	0	-2.751270	-0.780714	0.000253

Frequencies

237.8418	243.5161	379.2332
435.0964	441.7793	583.6393
642.0143	653.3240	696.9659
783.5136	857.3752	875.7191
939.8118	963.0958	973.3940
976.8006	1079.6210	1197.1707
1202.8788	1294.1164	1410.4091
1410.6228	1508.0734	1535.0769
2195.9656	3125.9506	3129.3132

3166.8511 3206.0760 3209.9608
T1 diagnostic: 0.01379522

C₂H₃

Geometry

6	0	-0.586593	0.029525	0.000047
6	0	0.706429	-0.142760	-0.000061
1	0	-1.039014	1.025199	-0.000132
1	0	1.602360	0.461323	0.000197
1	0	-1.282362	-0.807108	0.000020

Frequencies

712.2217	819.8520	921.4044
1045.9306	1391.0087	1650.4990
3039.2532	3134.3867	3231.4975

T1 diagnostic: 0.01697986

p5

Geometry

6	0	-2.265468	-1.080790	0.000148
6	0	-2.425763	0.281272	0.000180
6	0	-1.421096	1.319524	-0.000320
6	0	-0.017860	1.316623	-0.000050
6	0	0.913231	0.251298	-0.000002
6	0	0.220508	-0.997006	0.000331
6	0	-0.900927	-1.469191	-0.000604
6	0	2.330524	0.435622	0.000224
6	0	3.242563	-0.561563	-0.000084
1	0	-3.103704	-1.763950	0.000813
1	0	-3.448608	0.651116	0.000637
1	0	-1.848435	2.317020	-0.000592
1	0	0.428531	2.310287	0.000052
1	0	2.674664	1.466782	0.000614
1	0	2.938612	-1.602827	-0.000466
1	0	4.304669	-0.353163	0.000009

Frequencies

103.7075	178.4944	188.0364
269.2600	339.1578	374.0334
391.6297	455.9395	504.7295
581.9078	619.8231	666.6347
706.0485	746.6435	807.5742
865.2569	875.2525	909.2024
958.8625	974.5623	993.4555
996.5253	1067.9924	1118.0956
1184.4495	1240.1436	1293.4769
1310.8855	1398.8592	1414.3819
1447.6298	1491.1497	1551.0592
1598.0624	2203.4705	3118.2492
3135.4019	3137.9493	3144.3935
3162.9262	3204.0939	3231.7379

T1 diagnostic: 0.01423895

p6

Geometry

6	0	1.997429	-1.101944	-0.342124
6	0	2.556232	0.164916	-0.048856
6	0	1.675786	1.212811	0.097882
6	0	0.230704	1.210301	0.015765
6	0	-0.730254	0.210177	0.079166
6	0	-0.416669	-1.197200	0.317198
6	0	0.862673	-1.511296	0.006553
6	0	-2.134164	0.622579	-0.029091
6	0	-3.182839	-0.196386	-0.169877
1	0	-1.133891	-1.859349	0.784083
1	0	3.625288	0.346065	-0.003742
1	0	2.112288	2.200377	0.224949
1	0	-0.182785	2.210551	-0.085787
1	0	-2.310740	1.694772	0.001970
1	0	-3.073690	-1.272386	-0.239053
1	0	-4.189857	0.196217	-0.242109

Frequencies

93.7699	146.3592	209.6874
259.5094	355.9356	398.9032
428.5255	486.7822	509.7237
554.1635	597.1686	673.4708
744.2668	776.9913	794.5545
881.9879	909.8388	942.2169
969.5940	978.8786	1017.3028
1028.7525	1030.7762	1200.5268
1207.8676	1255.4496	1325.0212
1352.2550	1382.7086	1421.4039
1452.0751	1491.0934	1560.5954
1667.7037	1811.9320	3127.4251
3137.9052	3145.4448	3148.6009
3165.5783	3186.7666	3228.9994

T1 diagnostic: 0.01892524

p7

Geometry

6	0	-2.070171	-0.932507	-0.000069
6	0	-2.312928	0.260624	0.000365
6	0	-1.648951	1.508276	0.000132
6	0	-0.272365	1.396856	-0.000040
6	0	0.604863	0.252557	-0.000222
6	0	0.260567	-1.166600	-0.000193
6	0	-0.949223	-1.803418	-0.000096
6	0	2.020371	0.589883	-0.000349
6	0	3.101470	-0.218127	0.000447
1	0	-2.138927	2.471960	0.000198
1	0	0.260987	2.345394	0.000013
1	0	-1.015519	-2.883363	-0.000108
1	0	2.223658	1.658314	-0.001125

1	0	3.050219	-1.299905	0.001489
1	0	4.096289	0.209325	0.000178
1	0	1.121496	-1.826984	-0.000485

Frequencies

39.4210	156.2981	256.4368
259.5250	305.1889	372.9613
379.6171	445.2633	517.2800
550.4313	665.7328	668.8148
673.9741	722.6625	770.9522
841.0508	863.7190	941.8080
945.9684	969.3260	1002.5967
1013.7666	1103.0833	1139.5422
1198.0649	1221.7828	1243.5455
1334.6542	1401.1786	1427.4595
1432.7545	1469.9323	1546.6201
1615.6900	2187.4393	3122.7734
3134.3821	3148.4435	3166.3043
3198.1202	3205.9067	3227.5578

T1 diagnostic: 0.01404070