

Supporting Information

Gas Phase Formation of 1,3,5,7-Cyclooctatetraene (C₈H₈) through Ring Expansion via the Aromatic 1,3,5-Cyclooctatrien-7-yl Radical (C₈H₉•) Transient

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Table S1. Peak Velocity (v_p) and Speed Ratios (S) of the Methylidyne (CH), D1-Methylidyne (CD) and C_7H_8 Beams 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_7H_8	445 ± 7	15.0 ± 0.2		
CH	1857 ± 19	13.2 ± 0.6	20.8 ± 0.4	59.5 ± 0.3
CD	1845 ± 21	13.5 ± 0.8	21.9 ± 0.4	57.8 ± 0.3

Table S2. Statistical branching ratios (%) for the reaction of methylidyne radical with 1,3,5-cycloheptatriene (C_7H_8) at the collision energies (E_c , kJ mol⁻¹) of 0 and 20 kJ mol⁻¹.

E_c	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13
0	66.99	1.39	0.01	0.01	0.00	14.07	0.43	16.63	0.01	0.25	0.07	0.14	0.00
20	64.29	1.54	0.01	0.02	0.00	15.30	0.51	17.82	0.02	0.26	0.11	0.14	0.00

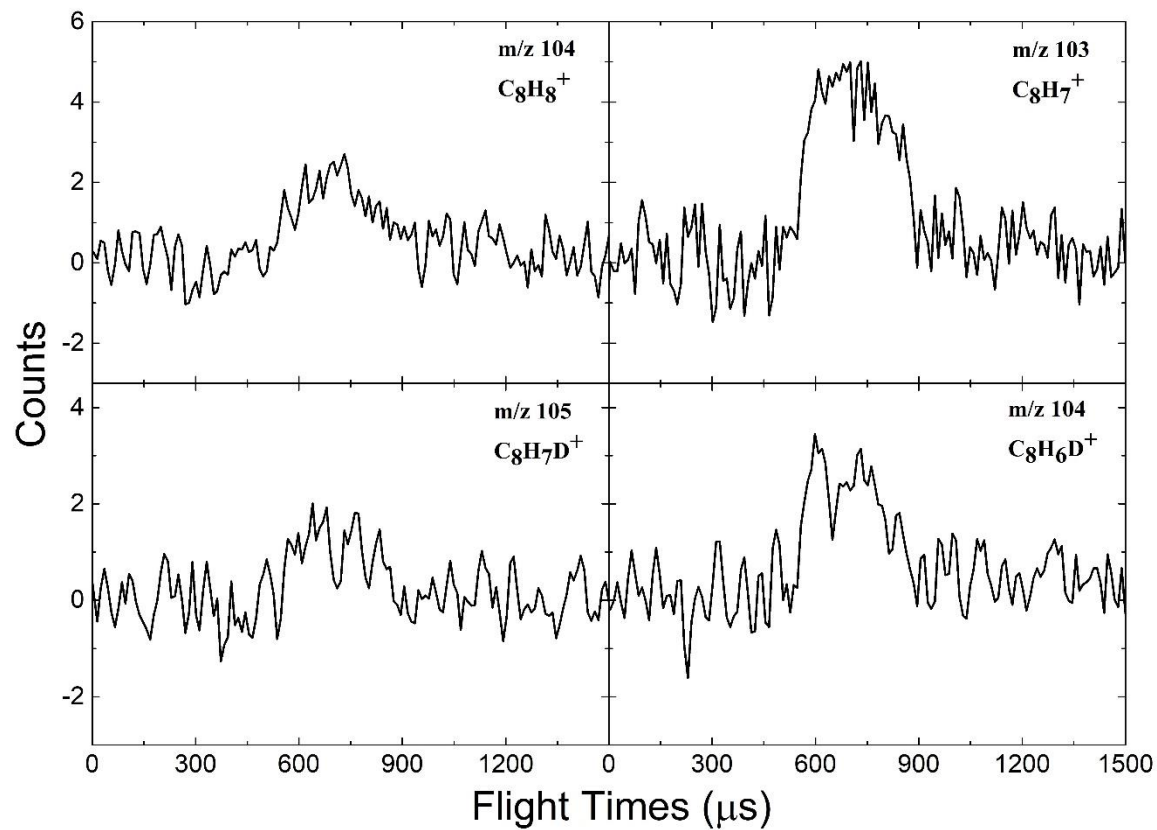


Figure S1. TOF spectra for the reaction of methyldyne radical (CH) with 1,3,5-cycloheptatriene (C_7H_8) and methyldyne-d radical (CD) with 1,3,5-cycloheptatriene.

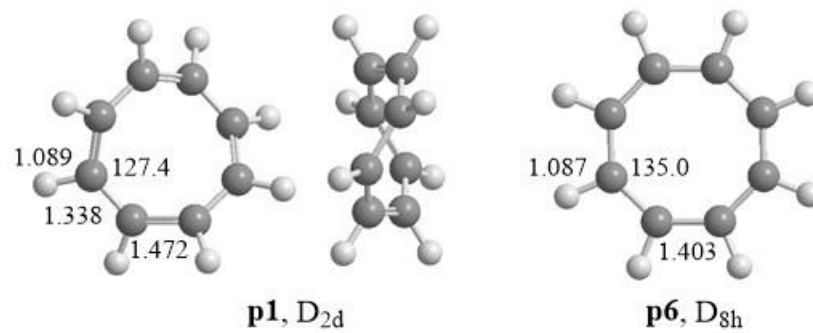
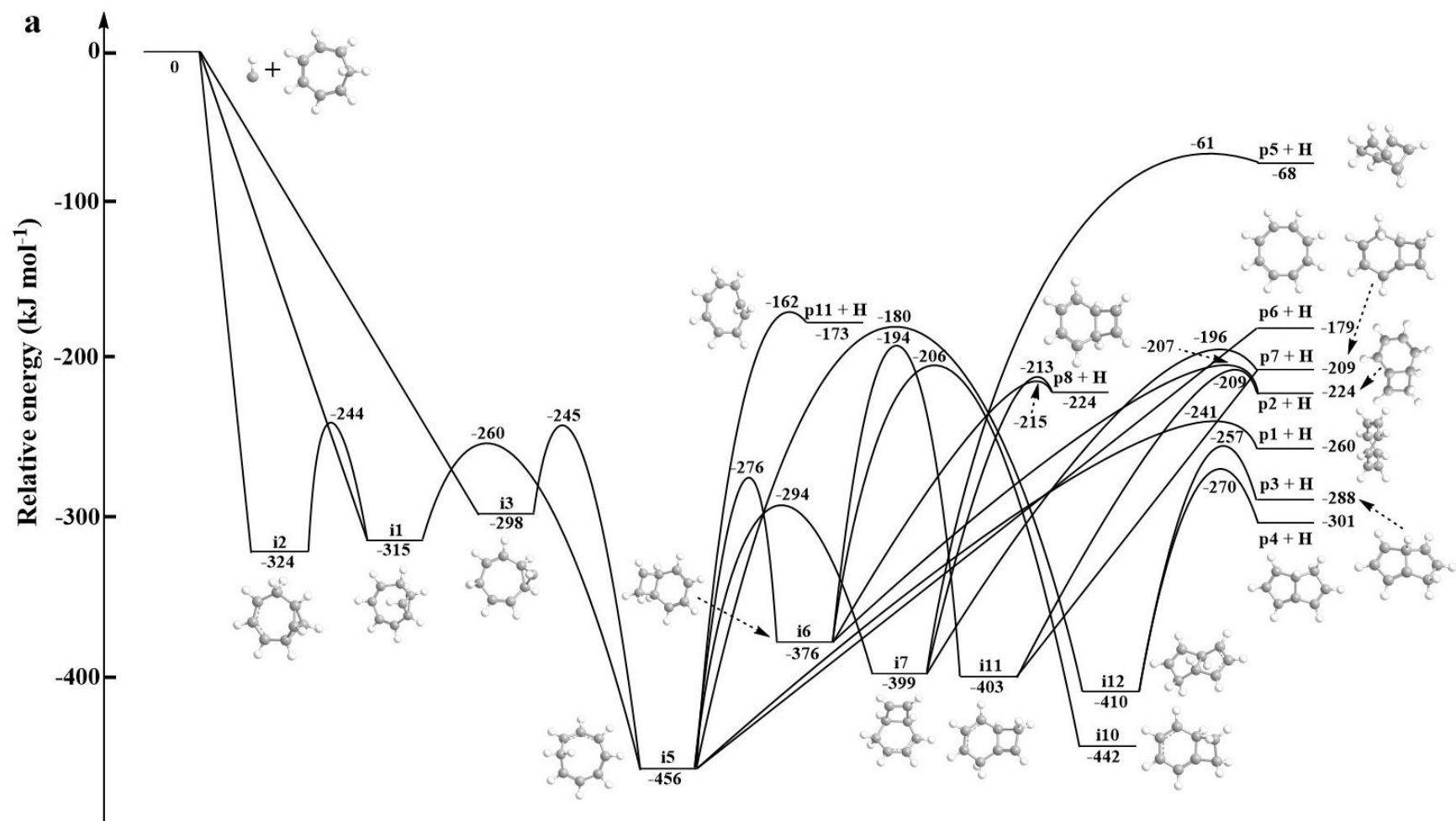


Figure S2. Molecular structures of **p1** and **p6**.



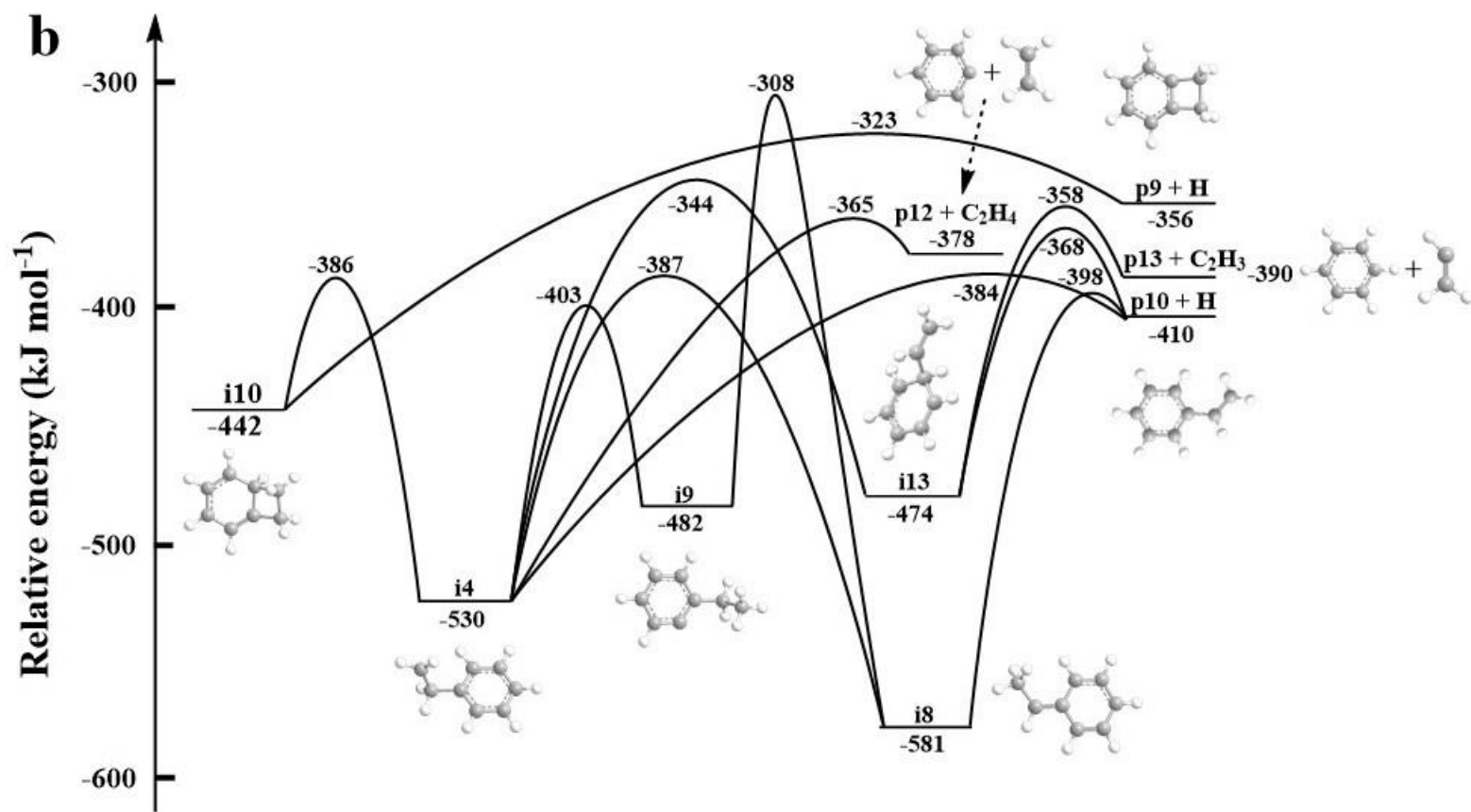
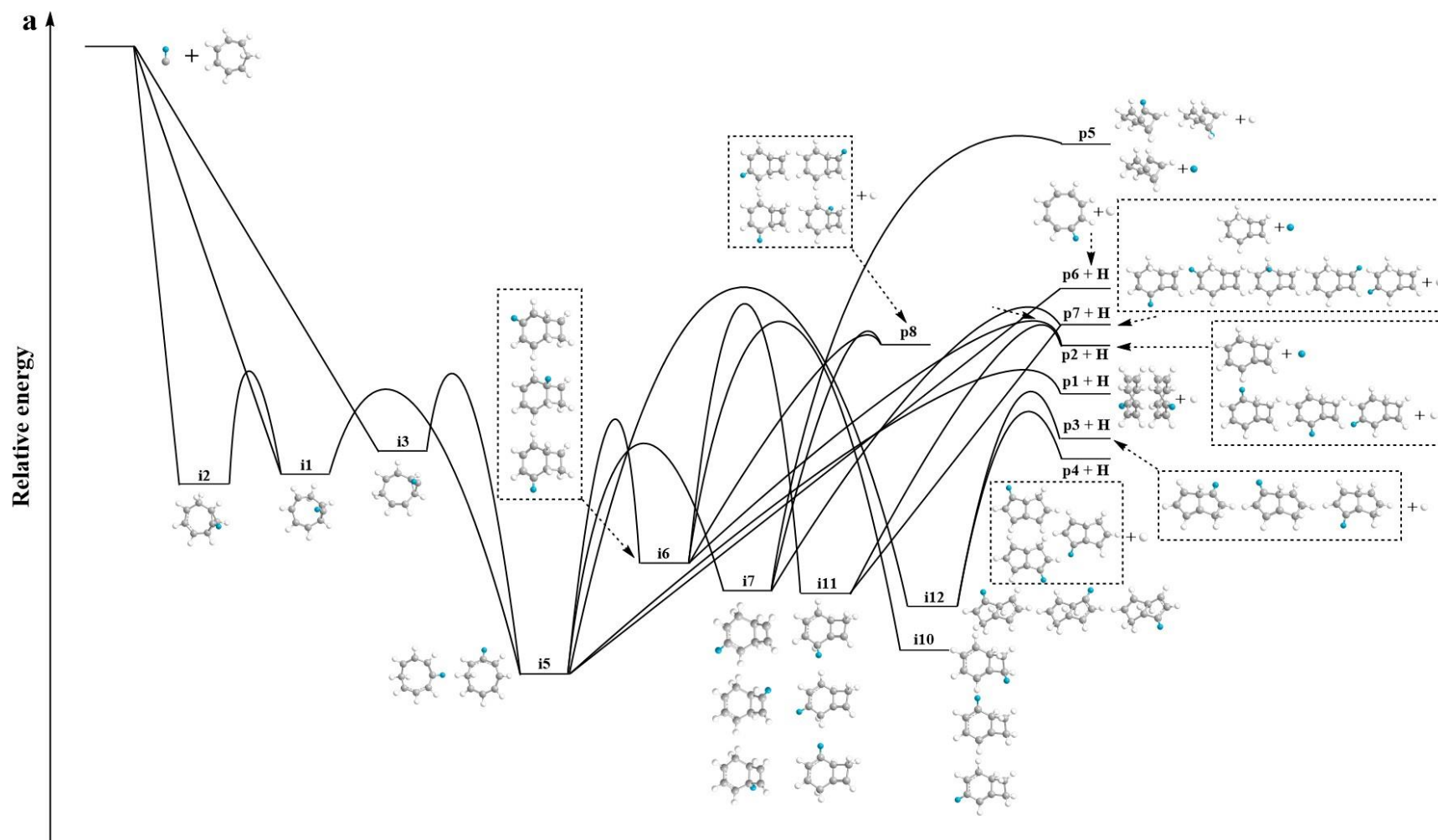


Figure S3. The complete PES of CH-C₇H₈ reaction (a) and the corresponding reaction pathways start with **i10** and lead to **p9**, **p10**, **p12** and **p13** (b).



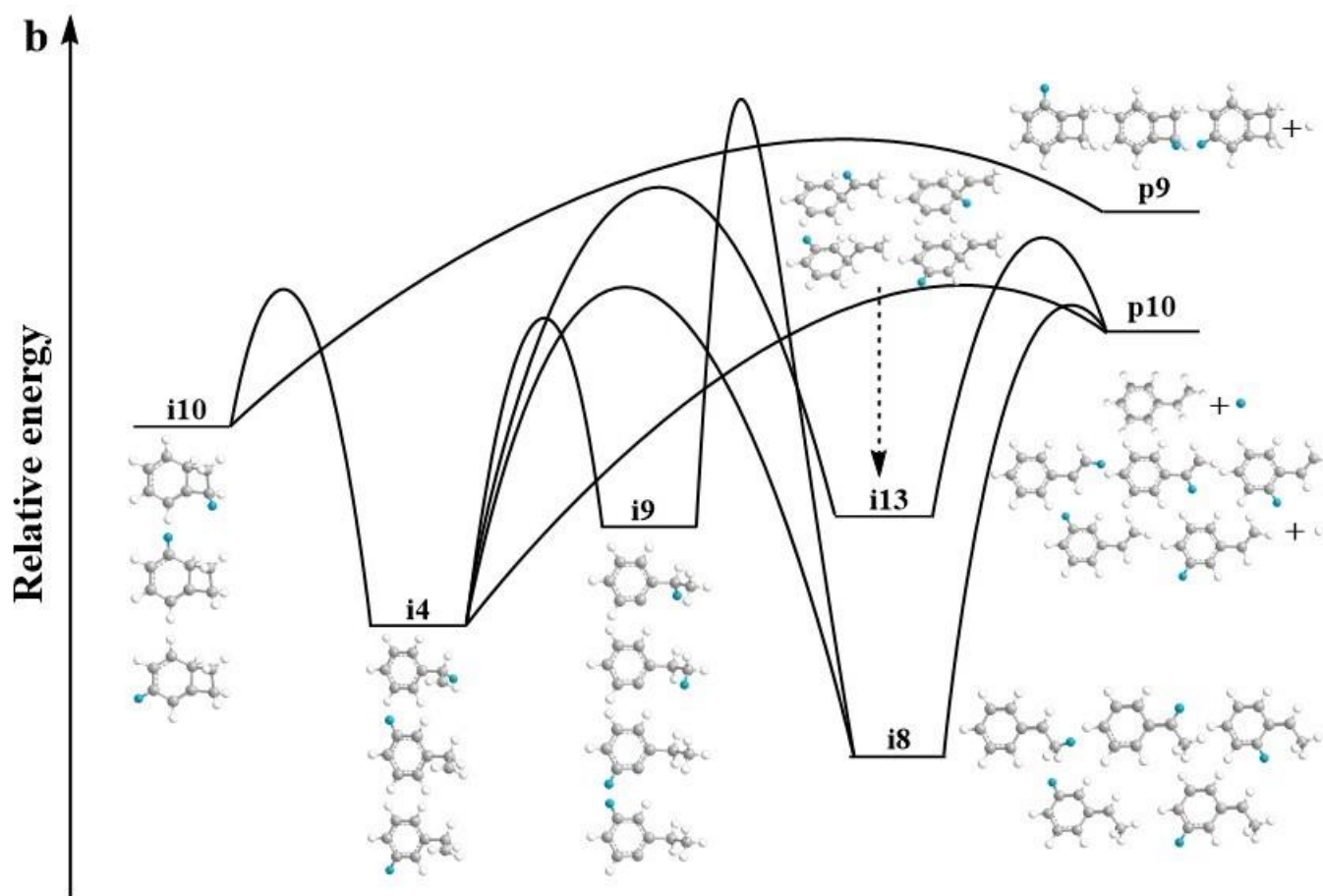


Figure S4. Atomic hydrogen or deuterium loss channels leading to **p1** – **p8** in the reaction of the D1-methyldiyne with 1,3,5-cycloheptatriene (a) and the corresponding reaction pathways start with **i10** and lead to **p9** and **p10** (b). Carbon, hydrogen, and deuterium atoms are color coded in gray, white, and light blue, respectively.

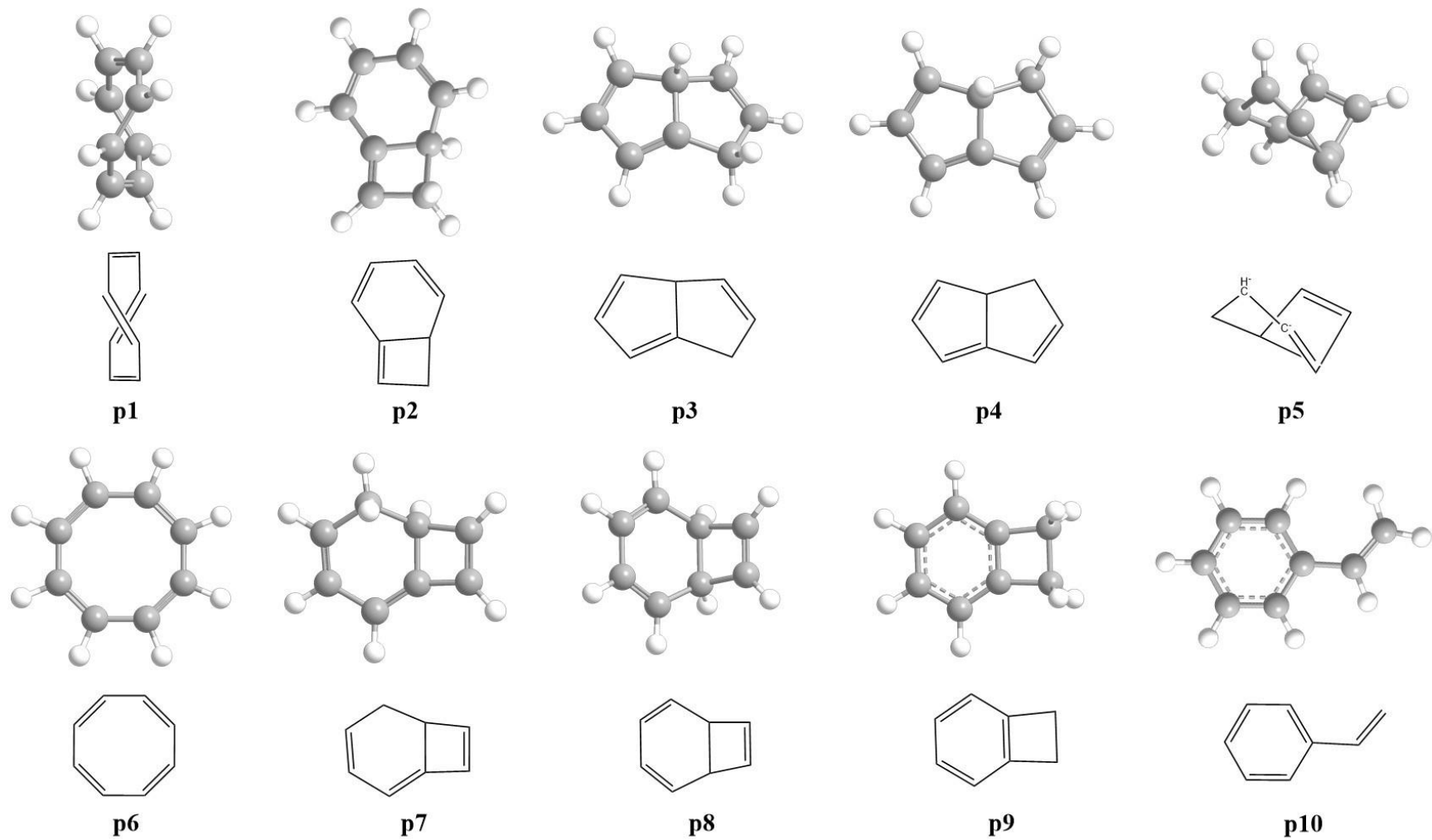


Figure S5. 2D and 3D structures of the products in the CH-C₇H₈ reaction.

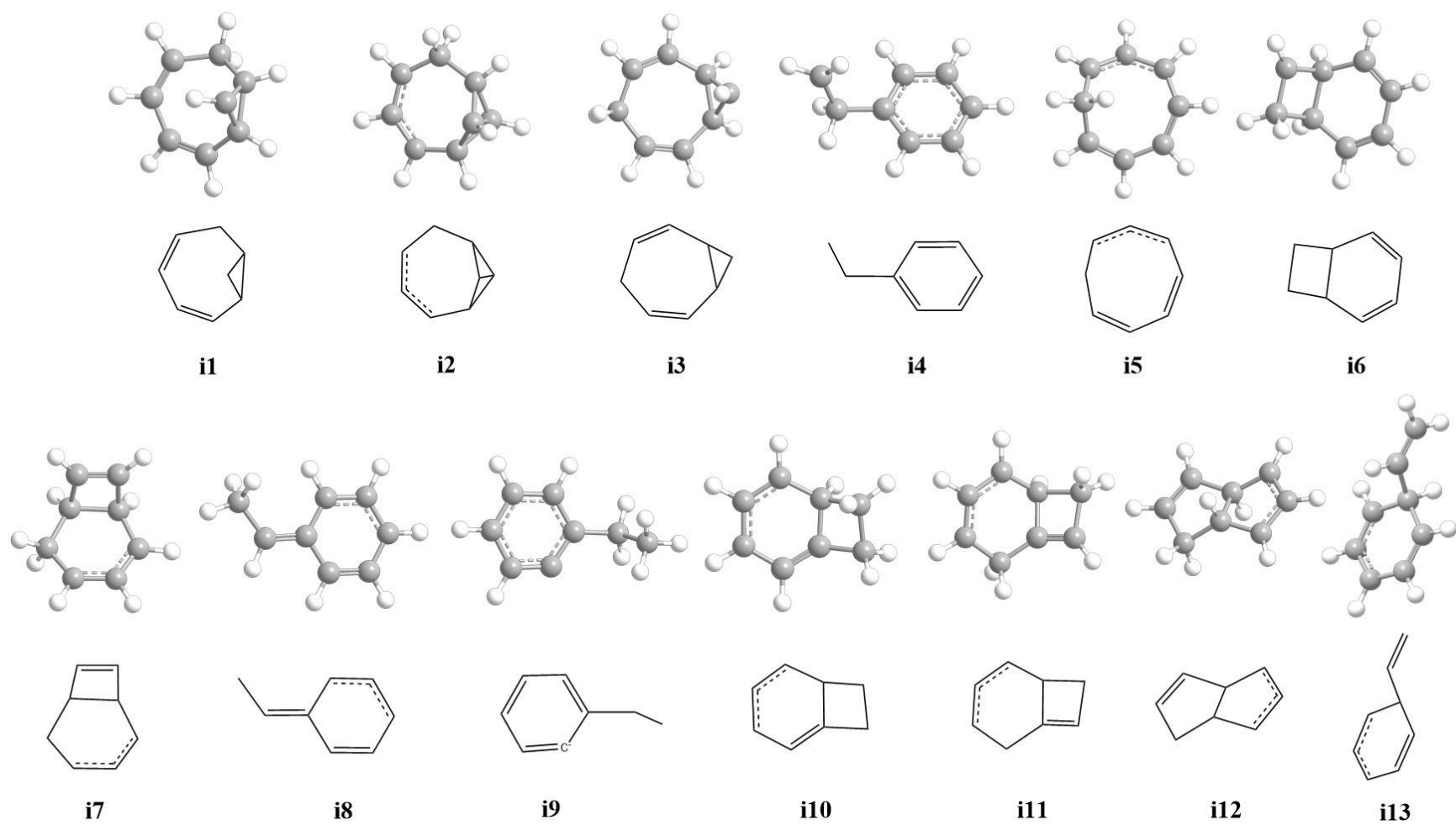


Figure S6. 2D and 3D structures of the intermediates involved in the CH-C₇H₈ reaction.

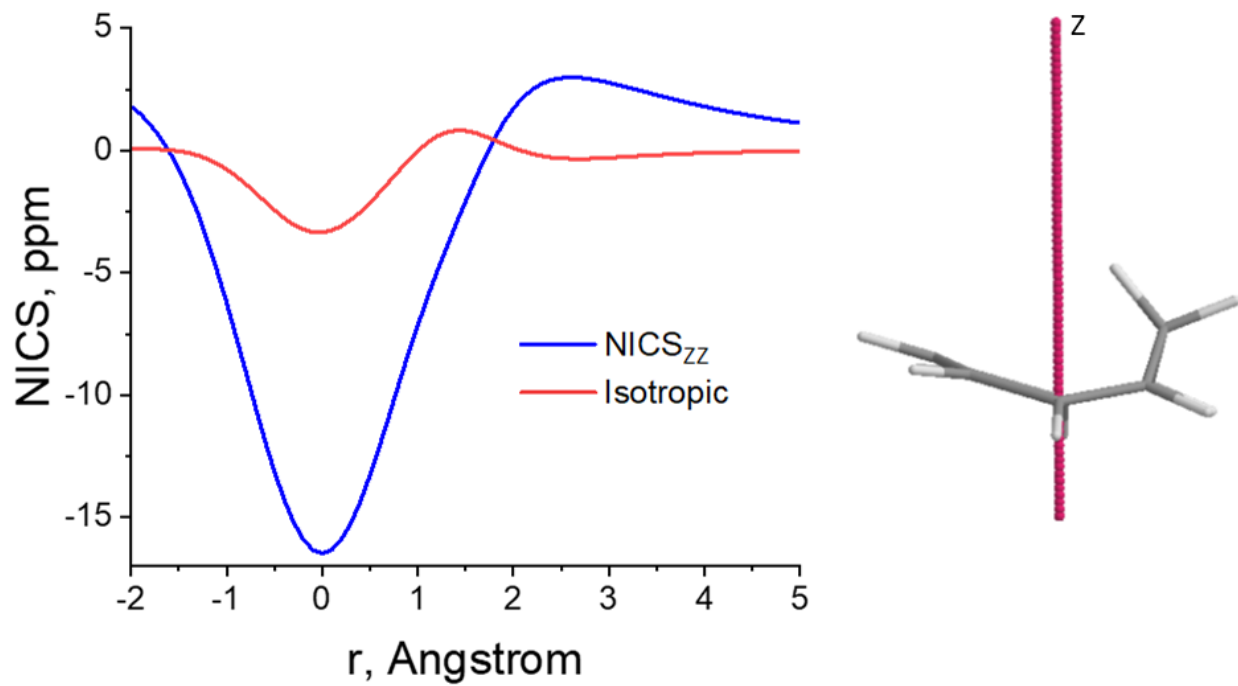


Figure S7. NICS value calculated at the GIAO-B3LYP/6-311G++(d,p) level for various positions along the z-axis.

Table S3: Cartesian coordinates and frequencies (cm⁻¹) of reactants, intermediates, transition states, and products.

Reagents:

C₇H₈

Geometry

C	0.962900	1.221662	-0.201833
C	1.461250	0.000004	0.528139
C	0.962908	-1.221657	-0.201830
C	-0.347692	-1.527396	-0.266295
C	-1.428573	-0.680788	0.186186
C	-1.428576	0.680780	0.186187
C	-0.347701	1.527394	-0.266293
H	1.689120	1.875474	-0.675651
H	2.550485	0.000008	0.591029
H	1.066596	0.000005	1.552847
H	1.689130	-1.875467	-0.675648
H	-0.635766	-2.475984	-0.712952
H	-2.365438	-1.177977	0.423881
H	-2.365444	1.177964	0.423882
H	-0.635781	2.475981	-0.712951

Frequencies

214.1530	295.1591	356.2739	417.4787	431.7858	610.3594
667.8505	725.3306	760.8684	813.1625	890.4729	921.0284
938.9040	960.3241	977.8923	983.2568	1001.3085	1040.0058
1067.7281	1210.2941	1221.3846	1247.3772	1269.1834	1327.3641
1385.7011	1424.3204	1475.5433	1480.5419	1573.1566	1663.2624
1671.0441	2993.2865	3088.7190	3124.8864	3130.8251	3137.5979
3152.2356	3158.6048	3163.3040			

T1 diagnostic

0.01109818

CH

Geometry

C	0.000000	0.000000	0.161152
H	0.000000	0.000000	-0.966911

Frequencies

2803.5760

T1 diagnostic

0.00842376

Intermediates:

il

Geometry

C	-1.187308	1.238375	0.139479
C	0.103557	1.547549	-0.571698
C	1.327264	0.716223	-0.178133
C	1.292322	-0.837697	-0.131199
C	0.061974	-1.630124	-0.338407
C	-1.220231	-1.267700	-0.133401
C	-1.748199	0.028356	0.285203
C	1.471769	0.002622	1.082580
H	-1.731760	2.092980	0.530434
H	-0.041177	1.421520	-1.654631
H	0.346621	2.604384	-0.422520
H	2.247539	1.080776	-0.636867
H	2.188548	-1.297839	-0.541232

H	0.235459	-2.656154	-0.652483
H	-1.969883	-2.043355	-0.268292
H	-2.728725	-0.009219	0.754677
H	0.846494	0.021286	1.964369

Frequencies

85.8421	220.9357	273.6507	371.0643	398.7674	442.2238
581.1541	638.8890	694.8989	715.8387	722.2026	817.1426
830.6514	857.8271	877.5157	926.0557	942.0445	990.8921
1000.0357	1016.0484	1024.0518	1057.9868	1086.1106	1099.8067
1230.0968	1244.8684	1260.5324	1273.3545	1331.0621	1365.9476
1410.8710	1431.2804	1462.3670	1482.9087	1651.4023	1694.7685
2981.4893	3044.8007	3068.1289	3101.6030	3119.9367	3131.1036
3148.9502	3155.3656	3204.6178			

T1 diagnostic

0.01283707

i2

Geometry

C	1.741634	-0.561699	-0.000080
C	0.646581	-1.581233	0.000129
C	-0.816408	-1.161063	-0.000275
C	-1.434858	-0.020819	-0.750534
C	-0.885399	1.172449	0.000186
C	0.523070	1.616727	0.000065
C	1.658768	0.814337	0.000042
C	-1.434961	-0.021100	0.750463
H	2.740784	-0.990073	-0.000243
H	0.796920	-2.241440	-0.868742
H	0.796506	-2.240661	0.869673
H	-1.454341	-2.047535	-0.000473
H	-2.287217	-0.037261	-1.414432
H	-1.577972	2.013930	0.000426
H	0.673107	2.692075	-0.000360
H	2.608992	1.343590	-0.000147
H	-2.287344	-0.038215	1.414311

Frequencies

137.1018	255.9201	378.7539	388.3098	422.8903	499.3800
632.1981	635.1331	710.1345	732.3814	734.5238	798.5348
854.9119	865.3035	895.9853	934.6936	944.4957	963.1873
981.5296	1016.4389	1022.9864	1083.1081	1161.1129	1179.3021
1189.7411	1225.1074	1250.8651	1254.5591	1321.9675	1384.6420
1408.4351	1429.5065	1458.4171	1480.5302	1500.0520	1536.4229
2961.5610	2971.3807	3069.7795	3094.8409	3121.4105	3141.3835
3159.0478	3192.4990	3205.9874			

T1 diagnostic

0.01534066

i3

Geometry

C	1.176431	1.323015	0.051398
C	1.889389	0.000029	0.028042
C	1.176454	-1.322974	0.051414
C	-0.109191	-1.641568	-0.113559
C	-1.284903	-0.771073	-0.338710
C	-1.284888	0.770984	-0.338849
C	-0.109216	1.641518	-0.113630
C	-1.886715	0.000066	0.772871
H	1.856827	2.156513	0.216459

H	2.551821	-0.000021	-0.853570
H	2.597087	0.000047	0.870016
H	1.856900	-2.156451	0.216376
H	-0.358080	-2.700279	-0.064502
H	-1.993269	-1.177585	-1.060395
H	-1.993163	1.177359	-1.060701
H	-0.358258	2.700187	-0.064372
H	-1.564023	0.000246	1.806828

Frequencies

79.2458	206.7706	265.0178	385.4404	386.1713	463.4068
469.8968	681.9926	699.0646	731.5064	777.9169	797.8263
822.9325	833.3882	866.6018	950.5102	950.9323	987.4337
999.1091	1015.1823	1026.5691	1065.0330	1077.7287	1106.1117
1231.1246	1241.9241	1267.9260	1278.9342	1357.9500	1407.3487
1415.8309	1426.5941	1449.9835	1451.9943	1726.9894	1731.9566
2958.7512	2986.7063	3072.7946	3082.7746	3108.2057	3108.8552
3131.2037	3133.6950	3185.2372			

T1 diagnostic

0.01251116

i4

Geometry

C	-0.343678	1.257333	-0.051926
C	0.481769	0.147921	-0.248454
C	-0.098352	-1.126140	-0.227184
C	-1.465027	-1.284874	-0.018828
C	-2.278505	-0.168916	0.175895
C	-1.713477	1.103048	0.159296
C	1.974155	0.306628	-0.469832
C	2.811977	-0.250363	0.634230
H	0.089171	2.252717	-0.064849
H	0.530309	-1.998467	-0.374631
H	-1.897077	-2.279638	-0.009640
H	2.258372	-0.167014	-1.418802
H	3.845315	-0.524029	0.458281
H	-3.343470	-0.291624	0.338158
H	-2.337270	1.977343	0.309863
H	2.196108	1.377579	-0.610708
H	2.445364	-0.254683	1.653142

Frequencies

25.4026	134.5795	146.3624	292.6706	355.6697	415.1538
476.0539	494.2898	574.5563	636.8668	715.2130	759.6459
780.8401	855.2714	859.8298	921.8061	976.8280	999.9542
1006.7615	1018.8345	1051.8319	1087.6556	1099.9284	1176.4002
1182.3260	1201.5075	1218.4881	1333.4786	1345.7589	1357.6962
1456.2973	1463.2565	1484.2662	1527.8665	1625.6588	1646.7777
2939.2880	3006.2554	3135.4629	3153.2858	3156.6768	3167.2720
3175.6381	3187.4544	3242.0978			

T1 diagnostic

0.01033472

i5

Geometry

C	1.255662	-1.261205	-0.148565
C	-0.001330	-1.495297	0.649079
C	-1.258086	-1.259072	-0.148352
C	-1.791393	-0.035621	-0.370183
C	-1.290059	1.248478	0.021907

C	1.292494	1.246191	0.022211
C	1.791287	-0.038761	-0.370285
C	0.001582	1.731977	0.254355
H	1.773553	-2.132804	-0.536483
H	-0.002156	-2.515336	1.040688
H	-0.000724	-0.812243	1.506605
H	-1.777756	-2.129728	-0.535990
H	-2.767876	-0.010341	-0.850529
H	-2.059515	2.012723	0.097885
H	2.063290	2.009037	0.098482
H	2.767731	-0.015348	-0.850818
H	0.002508	2.773910	0.569158

Frequencies

137.1302	195.0639	261.6417	302.1546	388.7014	446.0414
546.9004	581.4973	682.7685	688.1209	750.6415	766.8342
823.5946	854.4362	862.9033	921.1558	928.5511	960.9659
976.0709	987.5294	1051.7984	1060.3166	1183.1150	1213.1344
1272.5286	1272.7982	1284.5865	1316.7201	1387.0904	1411.8247
1435.3716	1486.2482	1488.0166	1527.6003	1615.7851	1619.9477
3016.6535	3073.9255	3107.8272	3113.7555	3118.0648	3135.3873
3145.3648	3158.2310	3162.6846			

T1 diagnostic

0.01262550

i6

Geometry

C	0.621718	-0.748485	0.588789
C	1.751216	-0.675530	-0.504948
C	1.687408	0.821936	-0.398077
C	0.561057	0.830017	0.606983
C	-0.732146	1.436191	0.119050
C	-1.720893	-0.782368	-0.238298
C	-0.639302	-1.449599	0.184010
C	-1.762510	0.682992	-0.284493
H	1.002715	-1.163730	1.525871
H	2.704192	-1.144817	-0.225884
H	1.455755	-1.087777	-1.479372
H	2.139105	1.614357	-0.984061
H	0.826046	1.276269	1.576974
H	-0.796028	2.520375	0.097897
H	-2.610341	-1.325222	-0.541323
H	-0.647134	-2.535202	0.230131
H	-2.673604	1.154820	-0.638327

Frequencies

64.5990	171.8994	256.1225	314.1283	428.7987	509.8973
561.7656	569.0220	710.5346	718.9339	774.6272	800.1031
832.8737	937.6531	955.9947	963.6027	979.9133	983.9263
988.2231	995.6866	1007.8302	1077.5253	1101.7916	1157.3980
1203.1247	1214.9058	1232.3521	1260.2871	1279.8476	1312.3308
1340.2877	1395.1902	1439.2737	1462.5305	1642.1788	1705.3383
2956.7267	2978.2084	3003.3154	3045.5913	3139.0237	3143.7386
3161.4340	3173.5331	3175.5596			

T1 diagnostic

0.01142475

i7

Geometry

C	0.619884	-0.836499	0.544517
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C	1.619120	-0.712524	-0.594902
C	1.760740	0.609283	-0.481159
C	0.724973	0.743895	0.643351
C	-0.503369	1.497589	0.252127
C	-1.731224	-0.507555	-0.396909
C	-0.765043	-1.442822	0.268966
C	-1.603863	0.867925	-0.310465
H	1.058948	-1.321415	1.423182
H	2.070641	-1.458330	-1.240758
H	2.363563	1.352178	-0.991092
H	1.136424	1.109675	1.591643
H	-0.478054	2.580517	0.322394
H	-2.611504	-0.935674	-0.864861
H	-0.652941	-2.361768	-0.319599
H	-1.205544	-1.766796	1.224936
H	-2.408842	1.485858	-0.698996

Frequencies

121.7504	169.5704	311.0066	386.3757	475.2754	524.7684
559.0769	620.3223	701.4028	743.7254	783.6181	808.6299
866.7619	909.4362	916.4885	953.5376	966.3609	977.7306
997.2805	1016.2451	1054.4751	1110.0117	1142.8802	1158.8902
1193.9061	1210.5054	1243.9966	1273.3050	1313.4533	1324.5754
1370.2055	1396.7042	1452.3163	1474.4903	1509.4037	1635.6744
2959.6234	3010.8220	3017.2722	3027.3333	3137.2622	3157.5655
3158.4778	3169.4373	3192.8502			

T1 diagnostic

0.01226287

i8

Geometry

C	0.540683	-1.307517	0.000000
C	-0.461247	-0.295279	0.000000
C	-0.015104	1.056472	0.000000
C	1.335720	1.363229	0.000000
C	2.298120	0.348925	0.000000
C	1.886259	-0.989164	0.000000
C	-1.830269	-0.645774	0.000000
C	-2.961349	0.331867	0.000000
H	0.229467	-2.347155	0.000000
H	-0.743590	1.858533	0.000000
H	1.648801	2.401849	0.000000
H	3.353262	0.596354	0.000000
H	2.626602	-1.781828	0.000000
H	-2.072621	-1.703529	0.000000
H	-2.936713	0.990017	0.878947
H	-2.937254	0.989367	-0.878947
H	-3.924833	-0.180160	0.000000

Frequencies

77.1843	121.7449	211.8924	238.3062	412.6659	429.5180
477.3035	561.5448	627.5703	627.9542	689.6822	767.7276
796.3897	828.7347	894.8752	971.2044	989.0720	989.6796
1006.8602	1027.8258	1043.2272	1072.8766	1129.0229	1175.8008
1188.6974	1244.6293	1327.8923	1350.9758	1403.7856	1426.4409
1480.9456	1484.7688	1492.0054	1506.5427	1580.6936	1603.2404
2987.5300	3018.6301	3100.8344	3153.6421	3159.3427	3161.6092
3172.3541	3183.4683	3190.7051			

T1 diagnostic

0.01577409

i9

Geometry

C	-0.324064	1.208604	-0.095640
C	0.455452	0.060336	-0.320854
C	-0.239728	-1.130175	-0.256353
C	-1.578714	-1.292070	-0.003744
C	-2.323977	-0.124465	0.216769
C	-1.690616	1.115735	0.168767
C	1.944562	0.132980	-0.579969
C	2.784070	-0.209924	0.661728
H	0.153578	2.183756	-0.135519
H	2.563413	-1.221203	1.012283
H	-2.048511	-2.269242	0.024089
H	2.201118	-0.555295	-1.390926
H	3.852749	-0.152748	0.436904
H	-3.387365	-0.192015	0.420442
H	-2.265094	2.020075	0.334950
H	2.196993	1.139218	-0.927995
H	2.571212	0.481328	1.481539

Frequencies

39.5594	132.9846	216.9030	305.3293	347.6594	419.5341
496.3933	562.6194	632.6506	706.6493	745.0922	774.9663
792.3889	852.9185	937.9525	972.1565	982.7896	990.1122
1039.9531	1056.6865	1081.9153	1138.5613	1173.5920	1216.3482
1250.3288	1302.0753	1325.4399	1353.6545	1408.9780	1449.4206
1474.2950	1492.0429	1496.9006	1509.2558	1574.1110	1634.1395
3026.7487	3032.1746	3064.2227	3092.3562	3100.2990	3145.2201
3159.0143	3171.7484	3184.6733			

T1 diagnostic

0.01173040

i10

Geometry

C	0.473589	-0.782516	0.434328
C	1.809989	-0.768341	-0.409521
C	1.968304	0.747705	-0.032469
C	0.494098	0.714027	0.293089
C	-0.608310	1.461595	0.028005
C	-1.920738	-0.621202	-0.133579
C	-0.819663	-1.414926	0.044032
C	-1.862186	0.798750	-0.081998
H	0.750721	-1.093518	1.458287
H	2.603095	-1.449203	-0.093851
H	1.607899	-0.895430	-1.473673
H	2.299783	1.438842	-0.810222
H	-0.536094	2.524976	-0.181705
H	-2.879161	-1.085724	-0.344743
H	-0.898617	-2.495675	-0.016397
H	-2.766941	1.373948	-0.237120
H	2.608819	0.871236	0.848092

Frequencies

141.2879	220.3086	346.1004	384.7356	502.3377	529.7183
568.4870	660.9393	684.6835	754.3156	761.6198	786.7785
864.1408	890.4203	902.0664	963.9197	964.0006	988.0119
1010.1311	1052.6165	1066.1736	1114.2576	1129.9441	1166.1950
1179.4911	1216.3840	1236.1341	1251.3415	1292.4744	1337.9231

1385.3353	1426.7053	1474.3669	1489.1679	1533.5959	1617.8405
2894.7296	3020.1322	3053.2977	3081.7592	3118.3230	3146.3255
3148.8440	3165.6714	3188.0148			

T1 diagnostic
0.01440663

i11

Geometry

C	0.681957	-0.647978	0.574554
C	2.066589	-0.482661	-0.173271
C	1.622951	0.954214	-0.411189
C	0.440876	0.800468	0.196753
C	-0.901305	1.442992	0.257296
C	-1.633268	-0.944019	-0.283022
C	-0.404451	-1.517878	0.034185
C	-1.923894	0.411348	-0.173421
H	0.827188	-0.827346	1.650136
H	2.956782	-0.645503	0.442549
H	2.146151	-1.086977	-1.081750
H	2.078263	1.771513	-0.960033
H	-0.954243	2.333233	-0.379919
H	-2.430373	-1.599102	-0.624429
H	-0.261690	-2.590298	-0.053264
H	-2.924465	0.760820	-0.403532
H	-1.134341	1.784747	1.278930

Frequencies

137.8620	203.3038	300.3383	367.3802	472.2179	503.0005
577.0553	609.8985	641.9538	713.1414	776.1422	827.9671
863.5077	900.9233	922.5899	947.7201	963.1238	968.4562
1009.2274	1042.6776	1101.2330	1121.8469	1139.2675	1153.6749
1187.3379	1202.5331	1226.9485	1273.5336	1285.3301	1328.4559
1381.8005	1439.5922	1460.9732	1477.4468	1489.0775	1709.2433
2953.6563	2970.1326	3026.4732	3030.3964	3071.7159	3138.1170
3160.0908	3170.7139	3173.1265			

T1 diagnostic
0.01072264

i12

Geometry

C	0.009470	-0.707397	0.249794
C	-1.394518	-1.175372	-0.158497
C	-1.357876	1.202150	0.091825
C	0.036561	0.742105	-0.273524
C	-2.161600	0.129085	0.092171
C	2.213910	-0.011599	0.026399
C	1.416166	-1.160762	-0.025972
C	1.446034	1.157509	0.050499
H	-0.048796	-0.604681	1.348053
H	-1.777620	-2.017348	0.423554
H	-1.445127	-1.453312	-1.221047
H	-1.679784	2.230163	0.204687
H	0.028841	0.670703	-1.381721
H	-3.237956	0.158414	0.218561
H	3.297601	-0.025717	0.048271
H	1.780049	-2.179613	-0.030960
H	1.833910	2.167078	0.074437

Frequencies

230.6255	254.9818	393.2374	430.9891	518.0180	542.2887
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597.5651	631.7001	657.3035	701.6876	747.6508	831.2368
852.2912	912.8565	934.0583	947.5855	957.5150	999.7028
1046.2174	1063.9352	1097.9715	1109.4525	1115.3562	1157.9369
1170.0600	1196.8641	1270.1375	1290.4780	1296.4288	1329.0156
1359.9221	1374.6467	1393.8721	1433.7033	1485.6910	1625.0257
2850.6416	2918.3141	2993.3216	3069.6354	3172.2517	3177.0303
3198.4816	3203.2256	3212.0828			

T1 diagnostic

0.01525709

i13

Geometry

C	0.242714	1.253277	-0.276342
C	-0.579993	0.000004	-0.454285
C	0.242708	-1.253274	-0.276344
C	1.561255	-1.223477	0.067239
C	2.250605	-0.000004	0.256130
C	1.561262	1.223473	0.067240
C	-1.773494	0.000005	0.493872
C	-3.046753	-0.000001	0.112516
H	2.099834	2.157404	0.194189
H	3.297776	-0.000007	0.531556
H	-0.269452	2.198999	-0.417710
H	-0.269464	-2.198993	-0.417712
H	2.099822	-2.157412	0.194189
H	-1.519819	0.000005	1.551543
H	-3.856068	-0.000007	0.834108
H	-3.327066	-0.000006	-0.936918
H	-1.005383	0.000006	-1.473403

Frequencies

73.1612	87.3149	260.5571	337.0728	371.7221	417.0508
553.8655	590.9230	620.4852	665.7871	677.2550	751.1988
791.3640	860.6064	939.0824	949.0722	969.2841	975.8095
988.9308	1014.8974	1015.0601	1035.7781	1110.4456	1114.1035
1172.7156	1197.1019	1262.2312	1291.9603	1315.9428	1347.3238
1396.7666	1441.0969	1449.4306	1539.1441	1597.6080	1691.0811
2914.2999	3122.1111	3137.1709	3150.8126	3152.9097	3172.4810
3172.7621	3193.8541	3207.7205			

T1 diagnostic

0.01457424

Products:

p1

Geometry

C	1.566321	0.665200	-0.375311
C	1.592230	-0.600559	0.375531
C	0.665437	-1.565832	0.375264
C	-0.600520	-1.591737	-0.375603
C	-1.566350	-0.665359	-0.375148
C	-0.665264	1.565867	0.375317
C	0.600657	1.591777	-0.375510
C	-1.592343	0.600598	0.375435
H	2.476449	0.888579	-0.930190
H	2.510274	-0.785965	0.931130
H	0.888171	-2.475982	0.930169
H	-0.785988	-2.510099	-0.930714
H	-2.476660	-0.888993	-0.929502
H	-0.888358	2.476064	0.930089

H 0.785976 2.510013 -0.930836
H -2.510865 0.786657 0.929998

Frequencies

178.5989	235.6806	263.6047	291.4661	363.7753	364.1265
649.6493	649.7514	673.9294	683.2940	774.5457	813.4009
813.5665	887.3365	941.5362	957.2126	957.3949	980.3771
1002.3253	1002.4276	1011.7957	1047.7173	1238.7615	1241.3691
1255.3776	1255.4595	1388.1344	1431.7521	1431.8573	1470.0035
1695.4833	1695.5476	1700.7636	1718.2828	3101.4408	3104.8069
3105.0978	3110.6471	3121.5151	3128.6674	3128.9544	3135.6720

T1 diagnostic

0.01153516

p2

Geometry

C	0.599302	-0.678294	0.494974
C	2.038578	-0.559597	-0.154710
C	1.722360	0.924906	-0.284706
C	0.459979	0.793275	0.169700
C	-0.830843	1.441768	0.142192
C	-1.726263	-0.830303	-0.230195
C	-0.556293	-1.469319	-0.034806
C	-1.888938	0.616926	-0.041582
H	0.702622	-0.874429	1.573502
H	2.884899	-0.849095	0.478800
H	2.116971	-1.084086	-1.109878
H	2.306687	1.761887	-0.649512
H	-0.943270	2.520217	0.169715
H	-2.603126	-1.391449	-0.537176
H	-0.482125	-2.545490	-0.163561
H	-2.889956	1.026284	-0.127093

Frequencies

190.3568	197.4781	368.4783	406.1248	506.9033	549.4640
600.5845	681.6754	709.2121	771.3394	815.1010	823.5453
875.1520	937.8920	949.6400	968.3917	984.2963	994.0882
1017.6815	1081.9412	1111.1035	1143.7706	1159.2056	1196.6082
1207.8622	1224.2199	1288.6717	1332.7177	1388.3773	1431.0977
1478.5667	1571.4769	1643.4037	1684.9874	2961.0401	3018.8054
3078.5883	3142.1892	3157.4419	3167.0733	3179.4433	3180.9256

T1 diagnostic

0.01133077

p3

Geometry

C	-0.020493	0.732431	0.302934
C	-1.472616	1.103713	0.149968
C	-1.159827	-1.234333	-0.204990
C	0.117244	-0.764677	0.467791
C	-2.032032	-0.229612	-0.336520
C	2.123306	0.147164	-0.252514
C	1.148747	1.244064	-0.119861
C	1.528136	-1.035594	0.001112
H	-1.631121	1.918674	-0.562657
H	-1.949965	1.407784	1.092772
H	-1.356095	-2.268094	-0.463302
H	0.078828	-1.053770	1.534140
H	-3.040890	-0.332347	-0.721096
H	3.160438	0.286554	-0.532943

H 1.335798 2.267025 -0.422785
H 2.008215 -2.004756 0.028356

Frequencies

162.9008	246.0116	376.8902	425.6761	544.1593	635.8962
669.5481	696.5986	708.7894	797.1880	835.1322	851.8418
889.2595	926.4301	949.8881	956.6880	967.8868	976.7530
1009.9017	1078.8669	1089.2419	1123.6753	1147.2572	1169.0072
1228.4892	1242.4816	1270.9956	1301.4076	1353.4262	1379.1259
1478.1435	1569.8705	1649.1425	1674.1307	2935.6722	2983.2862
3052.4045	3168.2077	3181.0004	3193.7951	3194.7711	3213.0471

T1 diagnostic

0.01114222

p4

Geometry

C	0.061473	-0.726704	0.407417
C	-1.276391	-1.185926	-0.243088
C	-1.369843	1.169846	0.094397
C	0.021586	0.770490	0.215787
C	-2.120482	0.076238	-0.141544
C	2.152115	0.065204	-0.192132
C	1.468864	-1.083474	0.019027
C	1.257591	1.225613	-0.094635
H	-0.025573	-0.929395	1.487057
H	-1.732953	-2.051315	0.245452
H	-1.122914	-1.449509	-1.294959
H	-1.737008	2.187736	0.130737
H	-3.194949	0.074857	-0.283241
H	3.211404	0.135023	-0.409601
H	1.890589	-2.078902	0.059280
H	1.541927	2.243772	-0.326093

Frequencies

188.0423	224.6151	394.3217	454.3423	547.9123	634.9304
666.1525	697.4957	737.0219	759.9358	834.5903	845.9143
868.3878	934.2688	950.8438	959.6764	964.0556	996.6000
1005.3596	1073.7267	1113.8858	1124.1221	1155.5166	1174.6277
1219.6741	1268.0942	1281.7310	1314.1429	1356.1523	1376.8616
1485.1827	1550.8271	1603.1904	1651.9586	2977.3512	3029.9281
3066.9614	3179.3863	3181.0070	3201.5795	3203.9823	3212.7365

T1 diagnostic

0.01138009

p5

Geometry

C	0.479240	-0.735711	0.715772
C	1.468317	-0.876047	-0.432927
C	1.656251	0.435552	-0.594446
C	0.717972	0.853818	0.524222
C	-0.590582	1.582089	0.234070
C	-1.540738	-0.448312	-0.699774
C	-0.963485	-1.255762	0.469957
C	-1.409953	0.842988	-0.486536
H	0.846716	-1.096737	1.683074
H	1.883253	-1.750697	-0.922262
H	2.267212	1.028978	-1.264930
H	1.220147	1.327503	1.374811
H	-0.859884	2.473867	0.789106
H	-1.763749	-0.914368	-1.652252

H -0.936190 -2.323410 0.231591
H -1.559641 -1.136828 1.378835

Frequencies

187.5097	223.4658	345.7915	367.7180	427.3382	540.8080
594.0791	676.7113	723.0764	742.7748	797.5034	842.7132
875.1227	883.0458	894.3304	927.4512	953.0190	1000.6875
1019.0720	1033.4598	1105.5151	1134.0396	1150.3877	1177.0341
1215.5954	1238.7214	1258.4220	1284.4768	1307.5758	1337.7885
1431.9923	1475.7268	1637.2445	1861.3602	3023.3793	3034.6838
3041.0369	3077.6802	3162.1926	3163.7151	3174.0765	3195.3340

T1 diagnostic
0.01186347

p11

Geometry

C	-0.485884	-1.327741	0.470616
C	0.485518	-1.327498	-0.470904
C	1.793504	-0.788575	-0.157270
C	1.780414	0.518333	0.210780
C	0.673386	1.472908	0.137160
C	-1.780266	0.518696	-0.210559
C	-1.793650	-0.788273	0.157290
C	-0.673022	1.473034	-0.137123
H	-0.208940	-1.421479	1.519132
H	0.208410	-1.419937	-1.519498
H	2.734611	-1.307746	-0.316124
H	2.737391	0.987932	0.430646
H	1.052363	2.487171	0.250587
H	-2.737165	0.988532	-0.430259
H	-2.734906	-1.307129	0.316340
H	-1.051766	2.487360	-0.250753

Frequencies

179.4590	200.4070	242.0241	346.5141	433.9380	447.5579
520.9755	631.0755	700.6690	712.5409	779.0603	798.0364
824.9716	841.2485	867.6008	916.7755	989.9352	990.6699
1003.0972	1015.3871	1061.6620	1122.8126	1192.7324	1230.6036
1285.2605	1306.4301	1370.9771	1428.0259	1429.9114	1488.1936
1507.4937	1611.4718	1625.1505	1633.7941	3097.6674	3113.6996
3115.0290	3119.6129	3124.9604	3133.7558	3148.8613	3151.3141

T1 diagnostic
0.01206774

p6

Geometry

C	-0.832714	1.632538	-0.000037
C	-1.743249	0.565406	-0.000021
C	-1.632538	-0.832714	-0.000103
C	-0.565406	-1.743249	-0.000171
C	0.832714	-1.632538	-0.000031
C	1.632538	0.832713	0.000168
C	0.565406	1.743249	0.000016
C	1.743249	-0.565406	0.000178
H	-1.326982	2.600523	-0.000065
H	-2.776853	0.901460	0.000005
H	-2.600523	-1.326982	-0.000158
H	-0.901460	-2.776853	-0.000309
H	1.326982	-2.600523	-0.000056
H	2.600523	1.326982	0.000274

H 0.901460 2.776853 -0.000013
H 2.776853 -0.901460 0.000322

Frequencies

144.4406	145.9957	330.3998	330.5897	451.5825	451.5826
599.7191	626.3545	739.0558	739.0561	758.0865	758.0866
763.7210	897.4723	898.2082	916.2960	916.2963	957.1123
957.1124	972.3119	992.2564	1210.7000	1210.7533	1303.3927
1303.3930	1363.4653	1451.9279	1468.5008	1468.5010	1498.1545
1498.1545	1568.5477	1569.4549	1701.7609	3115.8070	3120.7323
3120.7327	3135.2598	3135.6069	3151.6702	3151.6707	3161.3456

T1 diagnostic

p7

Geometry

C	0.551857	-0.718697	0.451909
C	2.012377	-0.624922	-0.001312
C	1.975035	0.719334	-0.160992
C	0.544799	0.783106	0.134656
C	-0.582760	1.480293	-0.055109
C	-1.859695	-0.614210	-0.043142
C	-0.587751	-1.409847	-0.306811
C	-1.837817	0.726474	0.071846
H	0.461137	-0.918314	1.525780
H	2.785864	-1.369059	-0.147971
H	2.709845	1.458501	-0.455741
H	-0.598607	2.522640	-0.356249
H	-2.796307	-1.153247	0.055789
H	-0.379457	-1.407460	-1.384914
H	-0.714766	-2.454035	-0.007769
H	-2.763991	1.271791	0.224812

Frequencies

196.7623	260.1524	300.8625	411.2856	487.1447	504.6784
614.7525	683.2785	727.5180	774.2097	792.8915	860.5948
878.9657	919.3505	938.7055	966.5897	971.8737	1009.4071
1020.6508	1049.4249	1102.5991	1127.2665	1172.8569	1201.4136
1211.1426	1294.1468	1311.7911	1324.3293	1361.9422	1405.5430
1473.7995	1548.4279	1625.0102	1721.8584	3001.2484	3025.8495
3064.3480	3147.2772	3161.8263	3172.8150	3179.4560	3207.8705

T1 diagnostic

0.01170665

p8

Geometry

C	-0.637536	0.795549	0.591868
C	-1.711188	0.668292	-0.484976
C	-1.710941	-0.668605	-0.485202
C	-0.637288	-0.795803	0.591676
C	0.644549	-1.445154	0.152231
C	1.697604	0.732211	-0.267987
C	0.644043	1.445256	0.152165
C	1.697893	-0.731766	-0.267892
H	-0.997624	1.238368	1.528158
H	-2.253800	1.415988	-1.053407
H	-2.252907	-1.416305	-1.054242
H	-0.997504	-1.238804	1.527827
H	0.690751	-2.530415	0.175657
H	2.598962	1.240287	-0.595502
H	0.689808	2.530539	0.175398

H 2.599506 -1.239533 -0.595184

Frequencies

161.6733	180.5108	375.4235	402.0013	533.5609	559.6140
589.6431	685.7587	751.2120	786.8373	804.5454	834.7112
912.9808	944.8869	960.3396	983.9402	987.0508	996.7664
999.1399	1018.1762	1046.5660	1118.9825	1162.5637	1200.1412
1221.6259	1225.9047	1293.4613	1330.0765	1332.3591	1397.0948
1441.5444	1628.7207	1642.9791	1704.2476	3005.1922	3016.2183
3139.0442	3143.1179	3158.1258	3161.1435	3173.6678	3190.6131

T1 diagnostic

0.01107070

p9

Geometry

C	0.000000	0.696591	0.452342
C	0.000000	-0.696591	0.452342
C	0.000000	1.436173	-0.718990
C	0.000000	-1.436173	-0.718990
C	0.000000	0.699791	-1.911899
C	0.000000	-0.699791	-1.911899
C	0.000000	-0.790950	1.972157
C	0.000000	0.790950	1.972157
H	0.000000	2.520749	-0.734978
H	0.000000	-2.520749	-0.734978
H	0.000000	1.223734	-2.861671
H	0.000000	-1.223734	-2.861671
H	-0.888434	-1.245988	2.417494
H	0.888434	1.245988	2.417494
H	0.888434	-1.245988	2.417494
H	-0.888434	1.245988	2.417494

Frequencies

189.5923	214.3787	401.0158	414.0336	487.5411	550.0285
646.1785	717.3905	728.5879	793.3040	795.3590	865.9125
880.5156	908.5149	944.3900	991.3739	1022.3055	1043.2919
1094.2076	1100.7781	1151.8105	1174.9357	1183.5810	1205.9793
1220.0410	1231.1743	1305.8018	1365.2260	1464.7649	1479.6455
1491.2310	1497.1589	1637.4733	1644.4470	3040.7029	3045.7679
3078.7522	3094.0431	3155.6755	3165.0093	3174.1779	3183.6919

T1 diagnostic

0.00996425

p10

Geometry

C	-1.006481	-0.421083	0.000000
C	0.000000	0.559025	0.000000
C	1.335345	0.129266	0.000000
C	1.658814	-1.224729	0.000000
C	0.648641	-2.182176	0.000000
C	-0.685795	-1.772245	0.000000
H	-1.478823	-2.511910	0.000000
H	0.895019	-3.237882	0.000000
H	-2.049073	-0.125287	0.000000
H	2.127682	0.870851	0.000000
H	2.699079	-1.530655	0.000000
C	-0.281556	2.003628	0.000000
C	-1.475086	2.602575	0.000000
H	0.604604	2.634724	0.000000
H	-1.553025	3.682939	0.000000

H -2.408753 2.051647 0.000000

Frequencies

11.4674	204.0380	236.2273	412.1962	447.2514	448.7270
560.6968	635.4811	655.6855	710.6330	787.3811	798.8247
850.0529	927.1512	928.5268	976.6978	998.9103	1014.9285
1029.1066	1040.2196	1056.5496	1111.8861	1182.5368	1204.5411
1226.2363	1318.0018	1345.7238	1362.2903	1451.6759	1483.1334
1528.9342	1618.3222	1644.5501	1690.4237	3129.0233	3143.8020
3157.2406	3163.7390	3173.2700	3181.8100	3190.3679	3223.5055

T1 diagnostic

0.01070014

p12

Geometry

C	0.000000	0.000000	1.396174
C	0.000000	1.223724	0.770601
C	0.000000	-1.223724	0.770601
C	0.000000	-1.211802	-0.631433
C	0.000000	0.000000	-1.322043
C	0.000000	1.211802	-0.631433
H	0.000000	2.157611	1.321577
H	0.000000	-2.157611	1.321577
H	0.000000	-2.150340	-1.175949
H	0.000000	0.000000	-2.406056
H	0.000000	2.150340	-1.175949

Frequencies

400.7984	426.7200	601.8083	620.3046	673.2115	721.2439
812.6919	892.3042	964.2640	988.7235	992.8273	1016.5033
1049.4246	1072.8390	1175.0928	1175.8042	1301.8397	1323.6091
1462.4597	1470.5076	1574.7712	1629.3472	3155.5943	3161.3592
3173.4439	3176.0825	3187.6436			

T1 diagnostic

0.01299069

C₂H₄

Geometry

C	0.000000	0.000000	0.663566
C	0.000000	0.000000	-0.663566
H	0.000000	0.922871	1.233870
H	0.000000	-0.922871	1.233870
H	0.000000	0.922871	-1.233870
H	0.000000	-0.922871	-1.233870

Frequencies

834.4832	971.9859	972.3758	1066.0797	1238.8796	1379.2185
1471.4392	1691.0568	3122.7317	3137.8212	3194.6631	3223.1010

T1 diagnostic

0.01050257

p13

Geometry

C	0.000000	0.000000	1.393968
C	0.000000	1.207153	0.696958
C	0.000000	-1.207153	0.696958
C	0.000000	1.207153	-0.696958
C	0.000000	-1.207153	-0.696958
C	0.000000	0.000000	-1.393968
H	0.000000	0.000000	2.478381
H	0.000000	2.146303	1.239146
H	0.000000	-2.146303	1.239146

H 0.000000 2.146303 -1.239146
H 0.000000 -2.146303 -1.239146
H 0.000000 0.000000 -2.478381

Frequencies

412.3852	413.3505	623.2294	623.2460	688.5182	723.2020
861.3635	863.1592	980.7396	981.8188	1013.0864	1016.4095
1023.3916	1060.1135	1060.4732	1174.6726	1197.4319	1197.6570
1334.7734	1381.7730	1512.7877	1513.0907	1637.1994	1637.2287
3155.4989	3165.1072	3165.1549	3180.8756	3180.9699	3191.5347

T1 diagnostic

0.01033130

C₂H₃

Geometry

C	0.048326	-0.585266	0.000000
C	0.048326	0.719173	0.000000
H	-0.879580	-1.164459	0.000000
H	0.968693	-1.165851	0.000000
H	-0.669027	1.526870	0.000000

Frequencies

712.3706	819.7887	921.5114	1046.3573	1391.4844	1650.7045
3037.6672	3133.6113	3235.4899			

T1 diagnostic

0.01523781

Barriers:

ts1: i1 – i5

Geometry

C	0.902465	-1.400138	0.223418
C	-0.226616	-1.331601	-0.766763
C	-1.473194	-0.712735	-0.164443
C	-1.034216	1.202739	0.010167
C	0.283697	1.569879	-0.385634
C	1.483085	0.971985	-0.095015
C	1.678416	-0.331766	0.492527
C	-1.493286	0.165921	0.940810
H	1.079197	-2.341743	0.733136
H	0.095639	-0.779433	-1.660453
H	-0.497122	-2.338391	-1.100795
H	-2.418895	-1.122698	-0.530570
H	-1.818627	1.868897	-0.344291
H	0.330814	2.498688	-0.949024
H	2.379977	1.547515	-0.312037
H	2.541989	-0.460221	1.141077
H	-2.415065	0.321684	1.492555

Frequencies

-615.1822	203.2566	236.1000	296.5755	336.1107	426.3834
496.0912	597.1988	612.2620	704.5752	753.2110	804.5734
819.4463	843.9061	875.7331	884.8277	896.5075	960.3964
967.5348	984.5190	1018.1251	1044.1390	1171.5189	1192.0206
1201.0676	1253.3311	1258.0732	1273.0058	1338.4208	1347.5666
1406.2377	1438.1685	1474.0004	1482.6796	1550.8729	1644.9520
2983.2374	3043.6734	3060.2758	3106.3878	3123.0143	3132.7604
3144.1999	3148.1996	3165.4234			

T1 diagnostic

0.01630364

ts2: i4 – p10

Geometry

C	0.419576	-1.274340	-0.033288
C	-0.473892	-0.207661	0.069261
C	0.039063	1.090487	0.121264
C	1.405395	1.314016	0.047497
C	2.285876	0.243593	-0.071155
C	1.788319	-1.052308	-0.108338
C	-1.928192	-0.482726	0.109408
C	-2.884149	0.351152	-0.345911
H	0.035207	-2.289019	-0.061423
H	-0.636678	1.930304	0.240886
H	1.788110	2.327431	0.093706
H	-2.200823	-1.513682	0.320881
H	-3.924676	0.050657	-0.354000
H	3.353973	0.419874	-0.126629
H	2.467502	-1.893151	-0.192644
H	-2.138966	-0.280019	2.035074
H	-2.655616	1.354325	-0.688284

Frequencies

-847.6613	60.5242	174.5487	236.9459	361.6775	388.4434
416.1110	452.1563	486.1584	569.8538	636.9025	644.8543
714.9694	791.7215	795.9951	862.1465	903.8136	940.0171
995.9092	1016.8331	1024.3077	1039.4590	1050.5640	1065.3999
1119.6845	1188.7444	1209.5561	1228.8017	1307.6758	1335.7291
1359.7953	1445.6669	1494.2945	1540.0834	1631.7991	1665.2597
1681.6851	3160.5333	3168.4282	3187.7665	3193.9859	3204.0779
3212.0353	3222.5056	3256.6032			

T1 diagnostic

0.01280667

ts3: i3 – i5

Geometry

C	0.368665	1.605349	-0.221795
C	1.326651	0.812206	0.643326
C	1.649060	-0.448240	-0.144047
C	0.815865	-1.482457	-0.457065
C	-0.568407	-1.547849	-0.111098
C	-1.742642	0.266770	0.007750
C	-0.959843	1.337585	-0.475306
C	-1.180082	-0.758195	0.892592
H	0.816203	2.413060	-0.792174
H	2.246960	1.386222	0.768627
H	0.952086	0.621182	1.645638
H	2.624609	-0.453364	-0.621991
H	1.180239	-2.214484	-1.173744
H	-1.219710	-2.055622	-0.822516
H	-2.723095	0.116539	-0.439864
H	-1.451376	1.994463	-1.189847
H	-0.681514	-0.519017	1.819728

Frequencies

-374.0722	156.9155	221.6918	319.3167	359.1325	370.4522
456.9889	542.0907	651.4149	658.9635	686.6842	738.0346
769.4920	790.9997	811.2549	888.5747	900.6440	967.4007
982.0268	1014.6297	1027.1770	1044.2439	1157.7356	1177.7744
1229.9819	1238.9765	1264.5892	1273.7053	1311.5157	1380.2647
1410.2891	1444.5677	1452.1805	1507.9268	1526.0564	1581.8825
3066.1265	3098.6982	3110.6617	3114.5837	3128.8998	3131.9680
3153.7399	3161.1861	3207.2604			

T1 diagnostic

0.01721775

ts4: i5 - p11

Geometry

C	0.332676	-1.310501	-0.512319
C	-0.627833	-1.198709	0.425753
C	-1.857533	-0.486782	0.098106
C	-1.673656	0.813566	-0.199836
C	-0.445297	1.614444	-0.086971
C	1.860469	0.330290	0.202566
C	1.699677	-0.954614	-0.170061
C	0.884213	1.429452	0.152194
H	0.054915	-1.341756	-1.563434
H	-0.350471	-1.265063	1.475568
H	-2.853933	-0.910397	0.169028
H	-2.556683	1.409753	-0.419685
H	-0.690850	2.673095	-0.149232
H	2.868231	0.663552	0.441183
H	2.555401	-1.613057	-0.284035
H	1.398026	2.380877	0.277368
H	-1.460932	-3.419878	0.596654

Frequencies

-361.0532	125.0294	185.6772	202.8436	206.4409	244.7377
349.3206	444.4154	453.5067	515.5968	644.3233	709.2898
723.6709	775.8785	799.5312	830.4606	847.6984	905.5207
919.7743	997.2567	1012.6737	1018.2517	1035.2233	1071.8972
1124.7992	1200.5225	1236.6464	1280.2153	1314.7827	1392.6751
1425.0203	1429.1193	1497.8647	1584.5107	1648.1617	1667.4110
1681.0927	3130.5929	3149.0859	3153.7481	3157.2909	3161.2118
3169.2916	3192.3506	3194.0489			

T1 diagnostic

0.01223178

ts5: i4 - i9

Geometry

C	0.637677	1.351019	0.000008
C	-0.431687	0.462157	-0.000024
C	-0.164856	-0.894543	-0.000037
C	1.107197	-1.425643	-0.000021
C	2.172660	-0.524775	0.000009
C	1.935515	0.847933	0.000025
C	-1.917686	0.760711	-0.000060
C	-2.598878	-0.607337	0.000080
H	0.467571	2.423436	0.000023
H	-1.488738	-1.328322	-0.000022
H	1.284752	-2.495353	-0.000031
H	-2.194629	1.350239	0.878975
H	-3.140339	-0.877764	0.904650
H	3.191959	-0.895900	0.000022
H	2.775006	1.534332	0.000052
H	-2.194603	1.350025	-0.879247
H	-3.140623	-0.877834	-0.904298

Frequencies

-1831.5796	60.9591	191.0103	349.1785	377.4864	424.0817
505.2488	513.2875	625.9145	678.1038	713.0676	749.5505
820.0539	839.9617	878.1754	953.2582	999.9699	1009.8237
1014.7287	1051.6358	1078.7379	1086.0873	1140.8848	1179.2410

1224.3182	1241.1724	1259.9800	1278.1961	1319.1355	1342.1965
1452.9934	1484.2817	1489.1368	1496.7256	1641.8976	1666.3293
1706.4375	3053.8624	3092.0973	3113.7832	3182.1410	3190.7472
3196.8013	3203.7976	3214.8523			

T1 diagnostic

0.01067672

ts6: i5 – i6

Geometry

C	0.445829	-1.063454	0.499830
C	1.294049	-0.843914	-0.767305
C	1.898893	0.423654	-0.269885
C	0.855646	0.963633	0.600528
C	-0.385195	1.535072	0.100051
C	-1.808873	-0.472530	-0.206399
C	-0.955008	-1.334067	0.420808
C	-1.483489	0.905093	-0.414196
H	0.995365	-1.573007	1.288682
H	1.990863	-1.660737	-0.982206
H	0.649441	-0.714430	-1.643520
H	2.946387	0.532251	-0.011908
H	1.228222	1.524773	1.464095
H	-0.481100	2.609349	0.257091
H	-2.849547	-0.752605	-0.337720
H	-1.363509	-2.185289	0.962652
H	-2.287238	1.538775	-0.777761

Frequencies

-631.8463	166.8814	226.5830	321.3754	358.8257	425.8831
519.7507	578.7961	626.7036	663.9809	712.2608	795.2328
849.7064	856.0983	890.8911	915.0750	966.2080	980.4941
995.5877	1011.3384	1041.2867	1068.7566	1110.9600	1141.1545
1165.6857	1214.9467	1249.6306	1270.2583	1318.9993	1373.6346
1396.6172	1430.6052	1475.8297	1483.7076	1535.7994	1633.5903
3015.9243	3039.1731	3050.4552	3101.2637	3109.6910	3129.2434
3146.5319	3164.7323	3171.5767			

T1 diagnostic

0.01424829

ts7: i9 – i8

Geometry

C	-0.382659	1.315456	-0.164995
C	0.407836	0.183820	-0.283723
C	-0.123592	-1.077964	-0.154313
C	-1.461792	-1.320946	0.094874
C	-2.267020	-0.183095	0.210104
C	-1.739648	1.103214	0.083986
C	1.839540	-0.200290	-0.516294
C	2.861270	0.084425	0.551790
H	0.015277	2.319936	-0.260346
H	2.489010	-0.219610	1.533635
H	-1.878542	-2.315553	0.197292
H	1.239414	-1.467292	-0.392500
H	3.802133	-0.434119	0.356261
H	-3.328361	-0.302260	0.401988
H	-2.405126	1.954012	0.181656
H	2.189869	-0.122968	-1.547070
H	3.072708	1.160131	0.600514

Frequencies

-2282.0355	118.7621	139.2332	201.9183	319.1014	395.6686
430.2790	515.0344	563.6208	638.4934	723.7173	768.6616
790.2411	822.4492	898.1120	968.3514	997.4487	1010.1158
1016.7755	1035.1610	1074.1366	1097.6254	1134.4640	1182.2055
1186.1149	1216.1484	1276.5228	1314.3775	1365.3172	1408.5807
1475.3000	1487.3777	1494.1491	1498.8418	1631.8633	1674.7598
1845.9801	3028.1241	3099.6703	3116.4327	3139.3339	3184.8835
3194.4035	3208.7984	3215.6766			

T1 diagnostic

0.01074803

ts8: i10 – p9

Geometry

C	-0.443044	0.713331	0.042314
C	0.721107	1.447263	0.004006
C	1.911756	0.711611	-0.016975
C	-0.446806	-0.689729	0.090487
C	0.735612	-1.424166	-0.050447
C	1.914910	-0.687572	-0.061464
C	-1.955122	-0.761646	-0.148681
C	-1.952698	0.805952	-0.031598
H	0.735699	2.530835	-0.033104
H	2.860817	1.235973	-0.036674
H	0.747389	-2.506451	-0.107783
H	2.866106	-1.204803	-0.122351
H	-2.206116	-1.111388	-1.152454
H	-2.425293	1.177994	0.880927
H	-2.552974	-1.301878	0.585180
H	-0.579553	-0.852536	1.911484
H	-2.360376	1.341982	-0.891071

Frequencies

-891.0089	183.1869	227.4621	358.5796	405.2050	445.6175
516.2185	526.1864	565.7802	643.1361	719.9390	734.2225
792.2113	805.2514	873.9020	883.9059	933.5420	957.5539
1004.7407	1029.0495	1041.1894	1104.5068	1110.7034	1161.8396
1179.6315	1194.2223	1214.4628	1228.5238	1238.5492	1308.5487
1365.5791	1464.8768	1478.7380	1491.1994	1507.6103	1637.4729
1661.2318	3077.0363	3090.3703	3129.7664	3152.1864	3190.2472
3200.5168	3210.8712	3219.0315			

T1 diagnostic

0.01240634

ts9: i4 – i13

Geometry

C	0.018352	-1.107445	-0.067177
C	-0.494380	0.233142	-0.099871
C	0.462137	1.299554	0.019257
C	1.814056	1.035528	0.072253
C	2.295939	-0.281772	0.050605
C	1.378975	-1.338577	-0.008798
C	-1.959825	0.528806	-0.028832
C	-2.983967	-0.363563	0.167226
H	-0.670161	-1.942194	-0.110689
H	0.103133	2.322825	0.055314
H	2.511652	1.862585	0.150463
H	3.359843	-0.478564	0.096048
H	1.738878	-2.362003	0.002863
H	-2.187960	1.590694	-0.052052

H -4.008378 -0.017147 0.169837
H -2.817931 -1.425911 0.287375
H -1.216797 0.415675 -1.227134

Frequencies

-1620.5087	125.4017	210.0783	225.5653	406.9771	410.2430
457.3916	548.9461	592.0529	623.7498	679.0885	725.4301
742.6979	773.0125	785.0079	848.4390	895.5127	965.1430
977.6438	987.6729	1009.8070	1031.0873	1096.0769	1114.6370
1171.2761	1185.7653	1201.1236	1273.2698	1317.9683	1350.7049
1422.6815	1436.9350	1477.8631	1494.8488	1557.0142	1567.6416
1626.2694	3146.3150	3155.8647	3157.0920	3162.7557	3173.3522
3188.5199	3195.7139	3245.1104			

T1 diagnostic

0.01900549

ts10: i5 – i7

Geometry

C 0.726330	-0.980698	0.652816
C 1.615114	-0.668116	-0.499786
C 1.556066	0.649130	-0.621752
C 0.695888	1.170535	0.497968
C -0.651111	1.498045	0.386685
C -1.552616	-0.619321	-0.475800
C -0.651615	-1.516524	0.354330
C -1.585450	0.726063	-0.403285
H 1.176801	-1.302619	1.590591
H 2.146319	-1.386557	-1.120278
H 2.037589	1.295274	-1.352086
H 1.244137	1.687079	1.287789
H -1.060829	2.259115	1.047417
H -2.315945	-1.126427	-1.059084
H -0.561369	-2.487829	-0.159464
H -1.169297	-1.741457	1.298012
H -2.413041	1.248743	-0.879947

Frequencies

-652.4091	137.8840	158.2200	288.9721	325.9208	382.1718
523.0788	535.8045	641.8126	658.3897	723.5381	749.3948
805.2676	856.9120	885.7885	908.1432	914.1362	953.8952
965.7598	984.4697	1010.6074	1025.4578	1098.2920	1117.2204
1196.7529	1213.5308	1222.6150	1298.8739	1331.6055	1372.1645
1385.1598	1433.7790	1459.2142	1474.4370	1625.8834	1697.3233
2942.8639	2988.6505	3085.1367	3110.7615	3111.0893	3119.6705
3128.7093	3148.9287	3151.2931			

T1 diagnostic

0.02047672

ts11: i7 – p8

Geometry

C -0.591790	0.845927	0.524092
C -1.679250	0.718010	-0.530350
C -1.779880	-0.607035	-0.421602
C -0.700149	-0.725083	0.643308
C 0.512497	-1.495190	0.214615
C 1.690151	0.548752	-0.427045
C 0.721405	1.368680	0.017824
C 1.588571	-0.901398	-0.311403
H -0.904018	1.380021	1.426515
H -2.173382	1.457445	-1.150493

H	-2.385633	-1.355554	-0.919905
H	-1.061887	-1.074174	1.616288
H	0.483109	-2.575330	0.325342
H	2.600169	0.968468	-0.842025
H	0.826931	2.444115	-0.087151
H	2.432943	-1.499595	-0.636805
H	1.612438	1.738632	2.011601

Frequencies

-436.5208	149.0303	174.5049	223.9521	292.7413	377.9433
430.5143	539.7423	565.6596	592.1745	705.4330	766.0057
807.6982	821.7900	848.0516	926.8559	961.9070	975.3970
992.7146	1003.1046	1014.2532	1017.1209	1030.4263	1058.9305
1137.3428	1174.4265	1206.4685	1226.3703	1237.0480	1305.7291
1338.1333	1353.5957	1405.5042	1453.5267	1632.6703	1661.4831
1720.4807	3056.4188	3071.4598	3173.0353	3178.7812	3194.9316
3196.5203	3206.8077	3229.8152			

T1 diagnostic

0.01187504

ts12: i7 – p5

Geometry

C	-0.806098	0.645458	0.618208
C	-1.650691	0.414004	-0.621553
C	-1.448879	-0.901543	-0.659138
C	-0.576615	-0.943554	0.578490
C	0.901101	-1.293470	0.482558
C	1.345033	0.837698	-0.586325
C	0.452128	1.529292	0.443986
C	1.553863	-0.413049	-0.245153
H	-1.368317	0.964012	1.502419
H	-2.226085	1.094812	-1.239036
H	-1.783881	-1.693947	-1.317852
H	-1.027681	-1.470563	1.425217
H	1.345590	-2.024779	1.147014
H	1.526506	1.266722	-1.563826
H	0.157630	2.525575	0.102083
H	0.959872	1.644793	1.405011
H	3.797314	-1.555646	-1.527464

Frequencies

-246.2045	26.2238	70.8218	187.8977	230.1250	349.2869
373.2730	432.6744	542.2660	600.5597	685.8736	745.5542
761.3542	814.6199	856.7593	888.7107	896.6195	913.8798
942.8452	975.1954	1018.4086	1035.1323	1044.6235	1121.9133
1141.2513	1163.8338	1193.4978	1234.7088	1251.2110	1274.6492
1289.1075	1325.6825	1353.3271	1446.8525	1477.8780	1672.0789
1896.4710	3059.3355	3071.7627	3077.4508	3118.2230	3194.8902
3202.2591	3209.2033	3229.8359			

T1 diagnostic

0.01164836

ts13: i7 – p7

Geometry

C	0.532713	-0.729948	0.462211
C	1.965091	-0.691416	-0.058150
C	1.965551	0.638662	-0.266400
C	0.547723	0.755675	0.092968
C	-0.571175	1.448149	-0.181215
C	-1.877480	-0.607078	-0.017855

C	-0.624905	-1.433466	-0.243965
C	-1.835781	0.734166	0.002006
H	0.477927	-0.887931	1.544335
H	2.708797	-1.464732	-0.207199
H	2.703876	1.347425	-0.617861
H	0.826417	1.617483	2.064271
H	-0.559392	2.465692	-0.555287
H	-2.822736	-1.121665	0.119619
H	-0.429057	-1.492532	-1.322156
H	-0.764719	-2.455917	0.115014
H	-2.751545	1.303708	0.121668

Frequencies

-536.1460	187.2234	217.8305	270.1810	305.2235	323.2371
417.6561	490.2374	500.3587	613.5587	686.1293	734.3081
788.9391	801.9855	857.6270	885.8913	939.8310	959.6591
988.6781	994.9873	1019.8689	1034.0776	1067.9236	1121.9955
1142.2572	1187.9979	1214.0043	1224.9727	1301.4378	1326.4753
1340.7118	1384.1272	1420.2226	1474.3684	1596.0875	1640.5495
1715.9093	3038.2472	3071.2548	3108.7004	3183.7057	3200.6767
3206.7608	3210.9771	3239.9152			

T1 diagnostic

0.01253034

ts14: i6 – p8

Geometry

C	0.650522	-0.734583	0.567589
C	1.693365	-0.528988	-0.531505
C	1.559681	0.810372	-0.551223
C	0.529111	0.851503	0.569134
C	-0.813504	1.404650	0.179587
C	-1.699825	-0.843346	-0.249354
C	-0.583108	-1.475157	0.136436
C	-1.818501	0.615258	-0.222401
H	1.055219	-1.155023	1.494231
H	3.531575	-0.684508	0.656658
H	2.223921	-1.233182	-1.161798
H	2.004385	1.595089	-1.153202
H	0.894509	1.321951	1.489736
H	-0.943802	2.482198	0.223298
H	-2.563999	-1.417775	-0.566904
H	-0.540731	-2.560702	0.142007
H	-2.767524	1.053701	-0.513595

Frequencies

-319.2393	141.4080	176.1158	229.2807	253.8510	386.4196
406.1476	535.4946	562.3893	589.5281	692.9284	755.0798
787.6290	805.7733	833.4010	912.5504	945.8998	955.5923
985.0667	986.1734	997.9847	1000.7835	1017.8451	1043.9431
1120.7321	1161.8453	1201.9593	1222.6358	1225.5109	1291.8502
1328.2157	1333.1032	1396.4310	1441.2558	1578.1274	1642.1567
1704.7651	3010.2961	3028.1092	3141.1061	3145.3395	3162.6579
3166.1867	3174.9602	3195.4447			

T1 diagnostic

0.01166790

ts15: i6 – p2

Geometry

C	0.594019	-0.689988	0.525107
C	1.989024	-0.632977	-0.217345

C	1.683785	0.836837	-0.442566
C	0.462620	0.780555	0.157455
C	-0.833921	1.433772	0.062564
C	-1.741631	-0.845655	-0.207900
C	-0.582788	-1.482037	0.042502
C	-1.891443	0.612411	-0.109282
H	0.740113	-0.870265	1.598543
H	2.870812	-0.879839	0.385286
H	2.013279	-1.228380	-1.134030
H	2.243403	1.633368	-0.919005
H	1.015576	1.709496	1.898634
H	-0.934023	2.512756	0.050703
H	-2.620427	-1.417049	-0.488871
H	-0.521635	-2.565186	-0.014865
H	-2.885091	1.027601	-0.239601

Frequencies

-541.1818	168.7002	199.7587	301.3053	327.7467	374.3524
413.0653	517.7179	550.4654	592.5424	678.2720	703.1991
765.4293	801.7747	820.4420	867.6122	940.7087	950.8657
968.6327	981.7858	995.4496	1007.3826	1073.2194	1109.4828
1151.7530	1157.7754	1200.5934	1211.5439	1224.1047	1286.2907
1330.8106	1383.6595	1428.5031	1469.6099	1573.1679	1602.3386
1673.3928	2991.8814	3016.9903	3069.9594	3142.9749	3160.2407
3171.2833	3182.2069	3186.7403			

T1 diagnostic

0.01241270

ts16: i6 – i11

Geometry

C	0.606814	-0.681642	0.511425
C	2.040287	-0.593345	-0.139422
C	1.779042	0.891473	-0.319477
C	0.466054	0.799881	0.149145
C	-0.858899	1.420982	0.027706
C	-1.738894	-0.863263	-0.204001
C	-0.530360	-1.473674	-0.061771
C	-1.948721	0.548304	-0.031869
H	0.695976	-0.859274	1.591324
H	2.874137	-0.893778	0.506634
H	2.117027	-1.147880	-1.082383
H	2.372946	1.699177	-0.726115
H	-0.046465	1.464620	1.166754
H	-0.946977	2.480506	-0.184882
H	-2.598341	-1.458036	-0.500109
H	-0.406101	-2.526124	-0.296229
H	-2.954136	0.948485	-0.065408

Frequencies

-1790.1161	170.0611	227.7473	353.8406	408.7418	515.0843
536.0127	559.8682	601.6139	687.1183	707.0878	742.2086
797.7311	855.9786	866.8852	946.4097	953.4836	958.2213
978.8195	999.8567	1060.5650	1080.9368	1113.6309	1140.2084
1161.2526	1201.3563	1212.1987	1233.7376	1266.3884	1322.0427
1363.2648	1411.2815	1438.5532	1473.7765	1510.3756	1579.3488
1722.6593	2978.7183	2997.8456	3032.5682	3142.5695	3164.0074
3168.8963	3192.0836	3198.2816			

T1 diagnostic

0.01588558

ts17: i6 – i10

Geometry

C	0.575337	-0.707302	0.522194
C	1.953193	-0.661481	-0.234515
C	1.826150	0.853588	-0.299543
C	0.435657	0.797890	0.257752
C	-0.826479	1.442234	0.071801
C	-1.778057	-0.807693	-0.207021
C	-0.611662	-1.458212	-0.008252
C	-1.920721	0.636034	-0.073031
H	0.720762	-0.957414	1.583584
H	2.819155	-1.099113	0.269126
H	1.867592	-1.100938	-1.237368
H	2.312527	1.625714	-0.881695
H	1.362521	1.271782	0.942898
H	-0.900992	2.521560	-0.005159
H	-2.655822	-1.370170	-0.510158
H	-0.539792	-2.532884	-0.146191
H	-2.906471	1.071119	-0.191349

Frequencies

-1876.4359	160.9153	186.5469	345.2289	418.9763	505.9727
536.4699	541.7590	606.3429	668.2075	707.3527	753.1754
784.0410	844.9217	910.7723	940.9254	952.0870	969.6260
978.3069	999.7530	1046.2330	1080.6538	1106.1891	1162.9816
1175.3728	1178.9563	1196.2717	1238.1097	1265.7958	1321.9157
1351.5402	1414.8178	1464.4054	1481.0800	1496.7423	1637.1364
2162.6706	2951.9211	2992.3422	3063.4533	3143.0879	3158.4251
3164.4672	3181.2509	3187.7957			

T1 diagnostic

0.01642345

ts18: i10 – i4

Geometry

C	0.522707	0.531754	-0.419511
C	-0.471161	1.402739	-0.073414
C	-1.768772	0.910189	0.187627
C	0.295664	-0.893373	-0.454428
C	-1.008933	-1.369423	-0.148820
C	-2.007046	-0.461985	0.180857
C	1.928698	-0.634662	0.700343
C	2.000935	0.619429	-0.166255
H	-0.248220	2.455203	0.068822
H	-2.566731	1.597948	0.441363
H	-1.227173	-2.429754	-0.200848
H	-3.002100	-0.828257	0.411323
H	1.568777	-0.483308	1.713401
H	2.605514	0.451026	-1.062379
H	2.667241	-1.424584	0.580765
H	0.910933	-1.500579	-1.115560
H	2.339195	1.534299	0.324725

Frequencies

-731.9686	163.8877	240.8249	360.0614	403.9699	538.7056
565.4867	596.0939	646.7514	728.6620	740.2327	789.8831
825.1209	836.6443	860.5891	926.8878	957.5033	985.3126
1009.5539	1011.0326	1034.2913	1051.7255	1102.1401	1171.1437
1183.2817	1196.6692	1201.5198	1266.2738	1321.0024	1357.7134
1453.8402	1459.0995	1491.0566	1513.5588	1568.8933	1646.8646

3064.5166	3113.0509	3118.9235	3129.5797	3187.3719	3192.3659
3208.9269	3220.2822	3226.6697			

T1 diagnostic

0.01776326

ts19: i4 – i8

Geometry

C	-0.495424	-1.288011	-0.007706
C	0.457245	-0.253989	-0.023036
C	-0.012297	1.068649	-0.027069
C	-1.373284	1.339853	-0.005183
C	-2.301363	0.306247	0.013503
C	-1.850941	-1.012353	0.007712
C	1.873164	-0.588728	-0.020301
C	2.985272	0.390067	-0.021534
H	-0.154925	-2.318951	-0.008808
H	0.689254	1.893982	-0.060933
H	-1.711754	2.370355	-0.010775
H	2.140800	-1.605752	-0.286109
H	2.793645	1.447254	0.088907
H	-3.363328	0.521960	0.028370
H	-2.564826	-1.828712	0.015194
H	2.502047	-0.306323	1.033780
H	3.974854	0.055777	-0.297948

Frequencies

-1886.1039	83.0948	188.7585	226.3190	371.4855	417.0330
433.5761	525.4929	551.6360	635.2185	638.8714	706.0692
746.5501	786.6255	820.1754	847.1377	911.0139	985.0154
1006.1539	1009.2177	1020.0830	1058.9401	1105.8853	1146.5775
1184.7070	1208.7915	1229.7183	1272.5175	1332.4085	1355.8138
1418.2765	1454.1067	1498.6592	1543.7158	1637.5191	1664.9942
2236.4467	3179.7471	3183.7248	3187.8655	3188.9371	3201.8547
3211.9002	3220.0383	3303.6678			

T1 diagnostic

0.01270524

ts20: i11 – p2

Geometry

C	-0.639494	0.640754	0.532346
C	-2.065898	0.518598	-0.119746
C	-1.689969	-0.931939	-0.377234
C	-0.445585	-0.788085	0.099482
C	0.874106	-1.384129	0.023175
C	1.649508	0.942962	-0.259405
C	0.464535	1.510966	0.024933
C	1.884237	-0.498325	-0.173415
H	-0.726091	0.760550	1.621750
H	-2.917622	0.714623	0.539590
H	-2.171292	1.116445	-1.027977
H	-2.230076	-1.754989	-0.829851
H	1.027793	-2.453057	-0.065204
H	1.107966	-1.742955	2.177869
H	2.485868	1.564267	-0.562342
H	0.338202	2.588075	-0.032997
H	2.896612	-0.857774	-0.321659

Frequencies

-525.6013	173.7684	184.5491	219.2579	262.9199	368.9672
429.1637	512.4281	551.8630	606.0117	694.2130	722.1224

787.0638	836.2327	846.5442	886.1541	951.8888	965.2971
982.0407	997.4129	1011.6467	1028.3093	1095.0361	1119.0165
1155.3908	1165.0845	1206.7855	1220.8592	1229.9359	1299.3225
1359.9590	1393.1983	1444.3094	1481.0932	1551.8498	1669.1243
1729.3404	3010.2714	3058.2091	3117.6488	3174.6071	3193.1675
3202.4396	3213.1238	3218.2097			

T1 diagnostic
-309.28660209

ts21: i5 – i12

Geometry

C	0.003528	-0.949102	-0.255538
C	1.341372	-1.200320	0.362567
C	1.366885	1.136231	-0.289444
C	-0.028690	1.207153	0.252186
C	2.104386	0.036543	-0.083040
C	-2.155956	-0.076306	-0.100646
C	-1.413474	-1.220388	-0.024346
C	-1.433790	1.149356	0.036572
H	0.152894	-0.751642	-1.318711
H	1.820744	-2.106007	-0.037795
H	1.307295	-1.303121	1.452241
H	1.838853	2.069306	-0.594795
H	0.102693	1.885775	1.119338
H	3.170900	0.001435	-0.283431
H	-3.240356	-0.077118	-0.129174
H	-1.843641	-2.217097	0.006708
H	-2.014947	1.999471	0.395754

Frequencies

-871.8614	183.2736	259.4565	356.9218	402.0475	459.7588
493.5103	545.6256	622.0323	668.6392	719.7422	762.5134
779.6964	828.0106	838.5634	887.6371	926.3419	936.9129
965.2508	987.7028	1018.9940	1052.1798	1119.5678	1155.1817
1166.5141	1212.0918	1268.5657	1281.4339	1357.3004	1371.9846
1386.5735	1426.4865	1443.6579	1466.8861	1514.4968	1637.1582
2876.5487	2978.0091	3044.4980	3067.1175	3089.4197	3109.8029
3146.6280	3164.1611	3176.2986			

T1 diagnostic

0.01459279

ts22: i12 – p3

Geometry

C	0.010253	-0.723817	-0.133156
C	-1.440678	-1.139465	-0.160267
C	-1.269590	1.225299	0.142751
C	0.083976	0.763811	-0.356381
C	-2.114423	0.187820	0.182331
C	2.185873	-0.066128	0.121966
C	1.276365	-1.209003	0.023903
C	1.504177	1.100512	0.020416
H	-0.099259	-0.532496	1.806327
H	-1.681941	-1.937436	0.545619
H	-1.749394	-1.487356	-1.157304
H	-1.535923	2.258695	0.325363
H	0.075610	0.911046	-1.456485
H	-3.171588	0.257545	0.410077
H	3.253661	-0.158795	0.276507
H	1.563214	-2.239903	0.184743

H	1.929909	2.094526	0.015778			
Frequencies						
-771.4264	229.8987	270.0324	379.3178	426.8065	457.7287	
545.6802	574.6299	612.1170	664.0154	683.5345	702.0430	
793.6737	832.5673	843.2784	868.6318	923.5745	939.8064	
950.9221	963.3941	975.6140	1007.6219	1073.0119	1096.6416	
1134.8423	1143.2431	1171.6423	1219.1233	1256.5827	1263.2498	
1301.0139	1355.9093	1378.6056	1467.6105	1521.0975	1606.2633	
1641.6806	2892.8981	2984.5480	3073.2056	3179.2457	3188.1626	
3204.6036	3205.0896	3219.1894				

T1 diagnostic
0.01348678

ts23: i12 – p4

Geometry

C	-0.043359	-0.732148	-0.335161
C	1.333287	-1.182629	0.211236
C	1.366874	1.176947	-0.123479
C	-0.030549	0.755165	-0.086449
C	2.148267	0.087287	0.010481
C	-2.188534	0.023275	0.076184
C	-1.459663	-1.119782	-0.018655
C	-1.329209	1.198410	0.012382
H	0.030842	-0.830890	-1.432211
H	1.756658	-2.056827	-0.289521
H	1.262968	-1.405561	1.283237
H	1.713162	2.199625	-0.195932
H	0.002151	0.594622	1.836234
H	3.231424	0.096421	0.023997
H	-3.264075	0.071136	0.193976
H	-1.853315	-2.126776	-0.040677
H	-1.662496	2.219109	0.141671

Frequencies						
-765.5047	230.6069	280.2351	377.4081	422.4293	461.2796	
546.9205	586.6675	617.9554	657.5089	686.3401	733.4722	
755.4794	833.8345	842.6878	861.4768	931.4706	943.7614	
953.6268	967.9402	994.8498	1008.8442	1084.6544	1110.5375	
1131.9996	1149.2340	1176.6473	1220.6974	1270.9910	1291.0333	
1311.3580	1344.3739	1378.2173	1469.7921	1502.6789	1583.6972	
1602.2650	2956.3970	3014.2476	3075.4718	3185.9310	3187.9173	
3209.8677	3210.4788	3218.5425				

T1 diagnostic
0.01418890

ts24: i4 – p12

Geometry

C	0.621321	-1.304428	-0.000152
C	-0.239861	-0.232425	-0.000025
C	0.154376	1.083608	0.000122
C	1.525371	1.343130	0.000144
C	2.435586	0.290427	0.000020
C	1.989883	-1.027669	-0.000129
C	-2.589051	-0.679954	0.000018
C	-3.228722	0.501020	-0.000006
H	0.260690	-2.328031	-0.000268
H	-0.573392	1.888231	0.000216
H	1.881737	2.368036	0.000262
H	-2.414264	-1.220808	-0.923291

H	-3.479756	1.008048	-0.925311
H	3.499637	0.497774	0.000039
H	2.705896	-1.842845	-0.000225
H	-2.414235	-1.220755	0.923353
H	-3.479729	1.008099	0.925277

Frequencies

-232.3864	40.2883	77.4484	87.4591	216.6581	327.4816
404.6683	439.2276	581.0392	613.3580	697.0074	730.7069
840.8714	846.0371	898.5157	909.2174	926.9269	987.3939
999.0654	1009.9520	1033.9849	1041.0103	1060.3791	1088.3656
1183.2591	1186.1598	1242.6099	1318.0830	1329.2934	1340.6849
1468.8518	1478.1181	1490.6708	1611.4498	1629.6317	1665.0740
3150.7459	3164.2020	3181.9449	3186.5314	3198.1883	3203.6035
3216.4255	3234.6573	3260.0465			

T1 diagnostic

0.01502313

ts25: i2 – i1

Geometry

C	1.698677	-0.653752	0.020326
C	0.559532	-1.615298	-0.077234
C	-0.877642	-1.132660	-0.061703
C	-1.436090	0.152009	-0.610412
C	-0.729331	1.372851	-0.198674
C	0.603222	1.611321	0.041829
C	1.706061	0.690810	0.043378
C	-1.527015	-0.158521	0.830639
H	2.667875	-1.144156	0.078917
H	0.688322	-2.177190	-1.012873
H	0.675563	-2.364071	0.718583
H	-1.551096	-1.961409	-0.295380
H	-2.259300	0.181602	-1.315264
H	-1.392542	2.230029	-0.103681
H	0.848378	2.629439	0.329618
H	2.682443	1.159896	0.134890
H	-2.344129	-0.154704	1.536288

Frequencies

-632.2704	128.3850	279.1856	334.5218	396.0994	422.5143
501.7991	592.9884	678.9590	730.0900	774.7156	786.1042
847.3409	877.5242	890.1720	919.0793	937.4649	961.5625
988.8968	1009.4655	1058.3412	1079.6138	1091.5710	1111.4865
1223.1447	1260.8307	1280.1869	1290.8201	1357.7914	1410.1973
1435.8047	1469.0944	1475.0870	1488.8613	1529.7539	1690.0616
3015.0087	3041.3074	3085.0141	3147.3444	3156.4742	3169.6761
3180.3871	3186.2355	3248.4133			

T1 diagnostic

0.01984843

ts26: i5 – p1

Geometry

C	1.714878	-0.090532	0.300305
C	1.292156	1.126150	-0.393633
C	0.090481	1.711231	-0.359020
C	-1.097399	1.287703	0.399370
C	-1.703495	0.101039	0.349984
C	-0.111543	-1.648068	-0.460794
C	1.070151	-1.275311	0.342563
C	-1.302250	-1.052280	-0.470021

H	2.676522	-0.026284	0.804698
H	2.083700	1.645468	-0.930519
H	-0.015599	2.662195	-0.877627
H	-1.555271	2.066314	1.006287
H	-2.622439	-0.026454	0.918266
H	0.021176	-2.537682	-1.072969
H	1.595235	-2.108507	0.802995
H	0.185285	-1.146979	2.181997
H	-2.086483	-1.487678	-1.085644

Frequencies

-708.8471	183.8124	220.6463	252.7026	291.9994	330.2825
357.5067	404.1289	419.2201	649.4865	654.1302	674.8501
712.0875	779.4243	818.3553	828.5604	898.5878	942.9272
959.3101	971.6509	997.6450	1013.9116	1020.9382	1032.3378
1057.7343	1239.3823	1244.0697	1257.9404	1263.7396	1384.3826
1432.4377	1435.1187	1480.5708	1656.4185	1720.2453	1736.9462
1757.0921	3138.3090	3148.2523	3149.9127	3155.0578	3162.6589
3171.2014	3173.9503	3180.1071			

T1 diagnostic

0.01321094

ts27: i13 – p10

Geometry

C	-0.011171	1.099988	0.171236
C	0.505786	-0.217756	0.212296
C	-0.395221	-1.283786	-0.029491
C	-1.748389	-1.049562	-0.177615
C	-2.245097	0.251559	-0.137841
C	-1.365955	1.321603	0.024541
C	1.963517	-0.486877	0.123523
C	2.874626	0.351723	-0.355940
H	-1.747984	2.336299	0.034678
H	-3.307468	0.432411	-0.251927
H	0.664079	1.935425	0.315687
H	-0.007858	-2.296216	-0.069889
H	-2.424786	-1.882052	-0.335351
H	2.272716	-1.472910	0.460700
H	3.920883	0.072883	-0.396324
H	2.613619	1.334463	-0.734247
H	0.548221	-0.381654	1.992416

Frequencies

-1053.0342	83.9242	181.7218	241.0528	398.6402	400.7385
462.6257	499.1730	512.3131	565.1466	631.1221	670.7521
701.1250	779.1009	808.1979	845.5999	935.5745	950.9429
991.3223	1011.1141	1012.8902	1029.7552	1043.7158	1056.7326
1122.1683	1183.8336	1201.8427	1227.3437	1308.7741	1338.0762
1358.7084	1452.3972	1487.2516	1518.9272	1618.7177	1653.6147
1727.3946	3161.0317	3177.3725	3191.9585	3197.5819	3208.0615
3216.6213	3224.6531	3250.8098			

T1 diagnostic

0.01355881

ts28: i13 – p13

Geometry

C	0.354875	-1.215019	0.572698
C	-0.297438	-0.000008	0.880171
C	0.354867	1.215011	0.572711
C	1.512063	1.207801	-0.183743

C	2.085777	0.000008	-0.584098
C	1.512071	-1.207794	-0.183756
C	-1.873916	-0.000003	-0.664117
C	-3.134652	0.000004	-0.305517
H	1.985439	-2.145111	-0.454832
H	2.993548	0.000013	-1.176368
H	-0.088133	-2.151987	0.889443
H	-0.088147	2.151972	0.889466
H	1.985425	2.145124	-0.454809
H	-1.394919	-0.000006	-1.635413
H	-3.943354	0.000007	-1.037507
H	-3.435221	0.000006	0.740711
H	-1.096516	-0.000014	1.613210

Frequencies

-470.4916	39.9737	85.1283	147.8686	212.8856	317.0517
385.3525	421.3733	619.0559	619.5975	683.1604	720.9229
829.3456	849.3409	886.1465	919.0093	943.6336	949.9354
993.5470	1001.9454	1015.6948	1033.0846	1054.5195	1063.7168
1106.7111	1173.9638	1189.3438	1201.8442	1327.8949	1376.4978
1401.9480	1498.9131	1514.9771	1619.9938	1631.9460	1666.3189
3087.6161	3164.9720	3179.6984	3186.6781	3189.8000	3205.2792
3208.4150	3216.7041	3222.9371			

T1 diagnostic

0.01558931

ts29: i8 – p10

Geometry

C	-0.501642	-1.286567	0.025969
C	0.445822	-0.258802	0.009878
C	-0.011663	1.063836	-0.000507
C	-1.368751	1.343897	-0.013846
C	-2.299894	0.310039	-0.011654
C	-1.861339	-1.007509	0.010799
C	1.874356	-0.602263	0.010887
C	2.894415	0.226679	-0.242024
H	-0.163674	-2.317954	0.045177
H	0.700187	1.881155	0.018836
H	-1.704460	2.374866	-0.018494
H	-3.360998	0.531537	-0.020236
H	-2.579412	-1.819645	0.019050
H	2.099711	-1.640565	0.243031
H	2.744184	1.256950	-0.545063
H	3.321373	1.133103	1.761549
H	3.915262	-0.135314	-0.240864

Frequencies

-432.3919	42.0115	143.1034	209.2703	252.2804	288.2421
414.8241	443.1841	474.6516	567.1772	638.3896	680.2940
714.1014	795.9538	806.0104	863.5752	939.6519	940.0035
998.1760	1015.2054	1023.1483	1029.7286	1049.4197	1068.0651
1125.5312	1189.0407	1213.7451	1238.7397	1323.0862	1347.4251
1367.3682	1456.6015	1495.4038	1542.3058	1648.9968	1679.2811
1687.6462	3158.3498	3171.3596	3184.7657	3191.8332	3204.1868
3214.6693	3221.8202	3257.9338			

T1 diagnostic

0.01131963