Supporting Information for

Barrierless Gas-phase Formation of the Phenyl Radical (C_6H_5, X^2A_1) via Atomic Carbon Induced Ring Expansion - A Versatile Framework to Hückel Aromatic Aryl Radicals in Molecular Clouds

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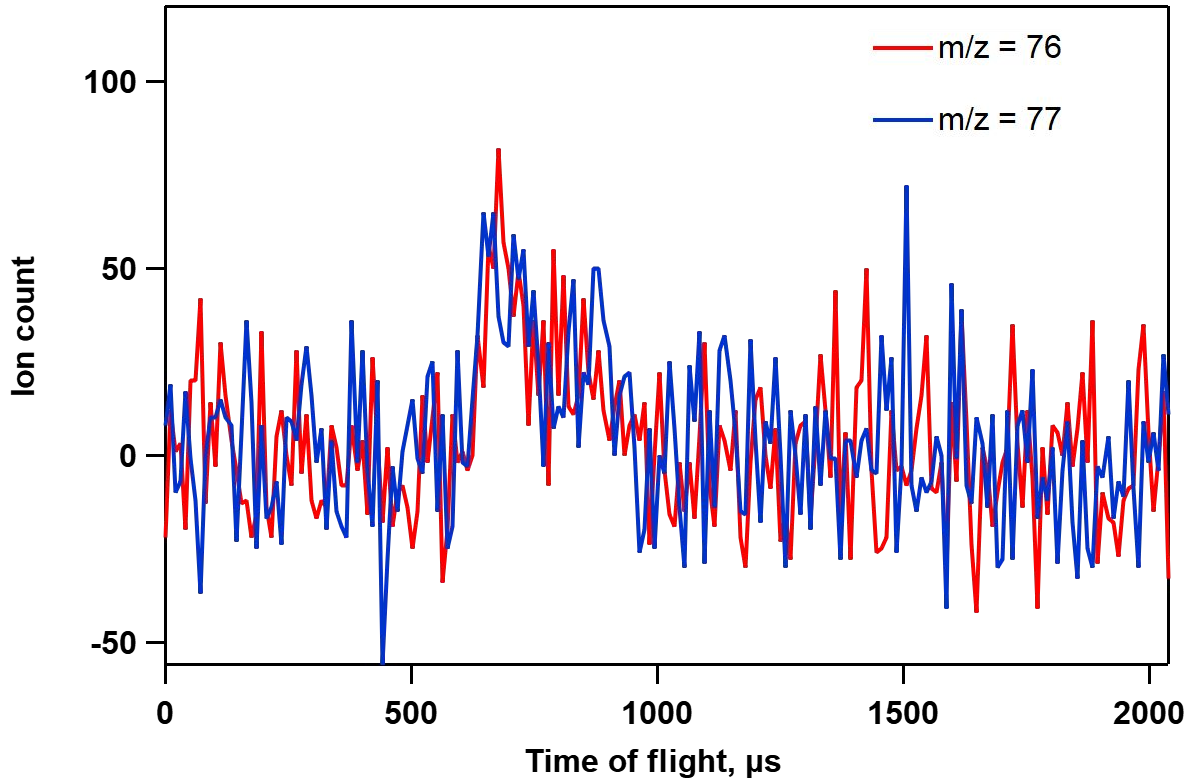


Figure S1. Time of flight (TOF) mass spectra for the reaction of ground state atomic carbon with 1,3-cyclopentadiene (c-C_5H_6) at *m/z* = 76 and 77.

Formation and role of intermediates i3 and i8

In order to explore a possibility of the carbon addition to the single C-C of cyclopentadiene opposite to the CH_2 group, we carried out the potential energy scan at the ωB97X-D/6-311G(d,p) level with C(^{3}P) symmetrically approaching the center of this bond (within C_s symmetry point group). This scan showed a monotonic energy decrease from the separated reactants to a bicyclic structure  where the attacking C atom takes the bridging position above the attacked C-C bond thus forming a three-membered ring attached to the five-membered ring of C_5H_6. This structure differs from the tricyclic structure of **i3** by the absence of the C-C bond between two carbons in *ortho* positions with respect to the CH_2 group. However, the bicyclic structure barrierlessly formed from the reactants appeared to have one imaginary frequency and to be a transition state rather than a local minimum. Intrinsic reaction coordinate (IRC) calculations from this transition state in forward and reverse directions lead to two mirror images of intermediate **i1** and thus, the bicyclic structure represents a transition state for isomerization between **i1** enantiomers. The barrier for this degenerate isomerization is 90 kJ mol^{-1} at the ωB97X-D/6-311G(d,p) + ZPE level of theory. Besides relaxation to the **i1** enantiomers, the bicyclic structure can further rearrange to the tricyclic isomer **i3** via a barrier with the energy 2 kJ mol^{-1} above the initial reactants. So, the minimal energy pathway (MEP) between **i3** and **i1** actually proceeds via the C_s-symmetric bicyclic structure and then bifurcates to the distinct **i1** enantiomers. No barrierless pathway exists between the separated C(^{3}P) + C_5H_6 reactants and **i3**; the MEP leads to the bicyclic transition state between the **i1** enantiomers and then to **i3**.

The other bicyclic structure on the potential energy surface, isomer **i8**, has a single C-C between two carbon atoms in *ortho* positions with respect to CH_2 and thus, the three-membered ring involves the CH_2 moiety. This isomer can be accessed by the ring contraction of **i5**, *i.e.*, by the formation of the C-C bond converting the six-membered ring to two fused five- and three-membered rings in **i8**. Interestingly, the C_s-symmetric isomers **i3** and **i8** can be formally connected by the formation of the C-C bond opposite to the CH_2 group. However, such a rearrangement appears to be symmetry-forbidden as the electronic term has to change from ^{3}A" in **i3** to ^{3}A' in **i8**. A search for an **i3**-**i8** transition state with broken symmetry was unsuccessful as **i3** tends to isomerize to **i1**, whereas **i8** tends to rearrange back to **i5**. Therefore, the MEP connecting **i3** and **i8**

is multistep: **i3 – i1** – **i2** – **i4** – **i5** – **i8**. The tricyclic **i3** and bicyclic **i8** intermediates represent 'dead ends' on the PES because H losses from them are highly unfavorable and cannot compete with their reverse isomerization to **i1** and **i5**, respectively. Thus, **i3** and **i8** do not affect the overall reaction kinetics.

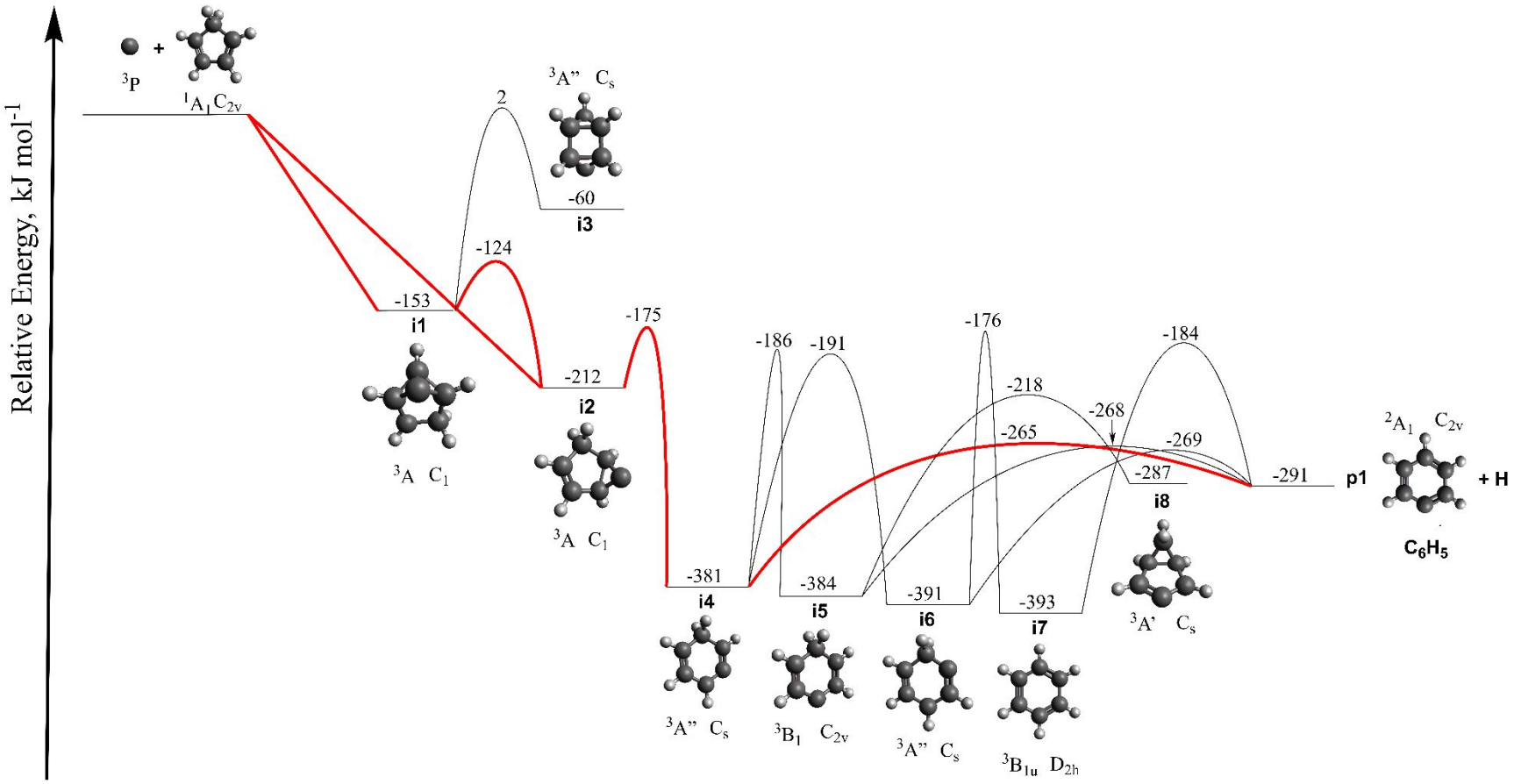


Figure S2. Extended potential energy surface for the reaction of carbon atoms (C, ^3P) and 1,3-cyclopentadiene (c-C_5H_6, X^1A_1) including **i3** and **i8**. Red color line represents the most probable pathway to **p1.**

Table S1. Experimental peak velocities (v_p) and speed ratios (S) of the carbon atom (C) and 1,3-cyclopentadiene (c-C_5H_6) reactants along with the corresponding collision energy (E_c) and center-of-mass (θ_{CM}).

Beam	v_p (m s^{-1})	S	E_c (kJ mol^{-1})	θ_{CM} (°)
C (^3P)	2028 ± 26	4.3 ± 0.2		
c-C_5H_6 (X^1A_1)	464 ± 9	17.6 ± 0.6	22.0 ± 0.7	52.2 ± 0.8

Table S2. Rate constants of unimolecular steps involved in the C + 1,3-cyclopentadiene reaction in s^{-1} at 0 and at the experimental collision energy of 22.0 kJ mol^{-1}.

	E_c (kJ mol^{-1})	
Step	0	22.0
i1 → i3	129.7	4.53E4
i3 → i1	8.40E6	1.05E9
i1 → i2	7.40E11	9.27E11
i2 → i1	7.49E9	1.32E10
i2 → i4	1.45E12	1.80E12
i4 → i2	3.33E7	6.62E7
i4 →p1	1.12E11	1.55E11
i5 → p1	1.38E11	1.91E11
i6 → p1	1.17E11	1.64E11
i4 → i5	1.74E8	3.22E8
i5 → i4	1.64E8	3.06E8
i4 → i6	2.27E8	4.11E8
i6 → i4	1.67E8	3.10E8
i6 → i7	1.50E8	2.99E8
i7 → i6	2.80E6	5.47E6
i5 → i8	6.48E8	1.05E9
i8 → i5	1.84E11	1.91E11
i7 →p1	2.24E7	4.43E7

Table S3. Contributions for the formation of **p1** from intermediates **i4-i7** in the C + 1,3-cyclopentadiene reaction at 0 and 22.0 kJ mol^{-1}.

Steps	Contributions of different channels, %	
	E_c (kJ mol^{-1})	
	0	22.0
i4 → **p1** + H	99.6	99.5
i5 → **p1** + H	0.15	0.21
i6 → **p1** + H	0.20	0.26
i7 → **p1** + H	2.0E-4	4.0E-4

Table S4. Optimized Cartesian coordinates (Å) and vibrational frequencies for all the intermediates, transition states, reactants, and products involved in the C + 1,3-cyclopentadiene reaction at the ωB97X-D/6-311G(d,p) level.

Reactants

1,3-cyclopentadiene (c-C_5H_6)

C	-1.174987	0.280323	0.000003
C	-0.733813	-0.986300	-0.000001
C	0.733535	-0.986524	-0.000001
C	1.175068	0.279992	0.000002
C	0.000168	1.212656	-0.000003
H	0.000278	1.870189	0.878579
H	0.000277	1.870188	-0.878586
H	-2.206003	0.606658	0.000004
H	-1.349157	-1.876796	-0.000002
H	1.348616	-1.877192	-0.000002
H	2.206162	0.606069	0.000004

Frequencies:

344.8194	528.7427	686.0802
727.3238	820.2107	821.0929
923.6599	937.8609	973.3638
975.3338	981.3630	1021.2779
1117.5129	1134.7098	1136.7786
1277.5036	1328.8545	1407.0279
1423.6326	1589.9256	1672.5359
3040.9139	3075.3875	3210.9332
3220.5675	3239.0491	3246.4486

Intermediates

i1

C	1.144055	-0.120553	-0.586258
C	-1.278828	-0.576669	-0.075945
C	0.418283	1.074897	0.045170
C	0.146283	-1.089986	0.104666
C	-1.044339	0.904495	-0.091681
H	1.865994	-0.263978	-1.375356
H	0.915061	2.035676	0.084898
H	0.389750	-2.145211	0.121940
H	-1.790706	1.666462	0.078333
H	-1.934632	-0.892731	0.745637
H	-1.725749	-0.954743	-1.006662
C	0.994592	-0.099763	0.829250

Frequencies:

206.2722	309.7284	474.0013
650.3889	703.0420	742.6043
772.6240	836.2249	845.4990
913.4655	941.0208	956.8427
974.2613	1020.8410	1041.4940
1058.7033	1128.3241	1155.6710
1224.1574	1279.5990	1291.0520
1325.3784	1446.2950	1457.9631
3004.3568	3041.6367	3208.5652
3214.8308	3240.0484	3248.0474

i2

C	1.380713	0.215420	-0.113345
C	0.740044	-1.145622	0.030873
C	-0.743614	-0.844368	0.244123
H	1.165991	-1.696359	0.876136
H	0.891828	-1.756611	-0.864824
C	0.532106	1.231481	0.030919
C	-0.870550	0.786236	0.260565
H	-1.471737	1.276678	1.024724
C	-1.464982	-0.082906	-0.740111
H	-1.272053	-1.391923	1.023289
H	2.438926	0.328237	-0.318820
H	0.804742	2.278531	-0.018647

Frequencies:

262.2556	394.4142	509.6980
620.5351	668.0067	744.1307
786.3676	879.0602	933.0930
948.2963	960.9845	969.5342
1011.0914	1033.5159	1050.4069
1133.2572	1182.6254	1197.3672
1265.3099	1314.2322	1363.8811
1398.4859	1483.3547	1687.8191
3048.8005	3087.7831	3120.7534
3128.7625	3198.3778	3224.4796

i3

C	0.642420	0.772097	-0.417379
C	-0.877143	0.810475	-0.207200
C	1.361616	-0.000171	0.644648
C	0.642196	-0.771823	-0.417844
H	0.959760	-0.000159	1.653295
H	2.441951	-0.000113	0.560803
C	-0.877009	-0.810706	-0.206908
C	-1.341133	0.000070	0.903252
H	-1.511402	-1.373764	-0.884753
H	-1.511255	1.374425	-0.884476
H	1.157838	1.415000	-1.117987
H	1.157435	-1.415038	-1.118296

Frequencies:

375.8423	393.8743	623.6779
652.9976	673.9517	767.3941
776.7860	820.2996	862.7949
892.4749	931.2703	971.4635
990.5906	1029.8699	1047.3312
1066.0192	1098.7548	1133.7778
1198.3272	1229.7735	1286.0187
1305.8014	1383.9105	1469.7846
3127.1408	3164.7579	3172.1591
3208.7885	3215.3617	3231.9252

i4

C	-0.014311	1.324307	-0.000009
C	1.204396	0.721623	-0.000028
C	1.333467	-0.695787	-0.000002
C	0.137141	-1.419549	0.000005
C	-1.109018	-0.939631	0.000022
C	-1.304039	0.559886	0.000011
H	-1.914053	0.854751	-0.869464
H	-1.914056	0.854764	0.869484
H	-1.986626	-1.577475	-0.000148
H	-0.079770	2.407074	0.000042
H	2.104050	1.329092	0.000023
H	2.304632	-1.173298	0.000065

Frequencies:

184.2271	392.5637	518.8843
549.0620	586.8668	642.5931
756.0379	774.0592	875.2847
929.8780	959.1749	976.6790
981.5878	1018.3303	1079.0819
1182.1259	1185.4291	1262.2234
1290.5338	1363.8145	1428.6342
1439.7268	1522.2538	1619.9950
2968.3749	2978.2401	3175.6609
3184.0306	3197.0602	3218.3916

i5

C	-0.000005	-0.807459	1.241644
C	-0.000005	-0.807459	-1.241644
C	-0.000005	0.555137	-1.260500
C	0.000081	1.372202	-0.000000
C	-0.000005	0.555137	1.260500
C	0.000026	-1.456504	0.000000
H	-0.000109	-1.372397	2.167902
H	-0.000109	-1.372397	-2.167902
H	-0.000016	1.086297	-2.206776
H	-0.867395	2.052720	-0.000000
H	0.867123	2.053156	-0.000000
H	-0.000016	1.086297	2.206776

Frequencies:

166.9921	372.0504	521.4741
561.5637	577.3828	706.6201
728.2103	873.4092	926.2449
956.6576	959.4769	960.1272
972.9724	988.6889	1162.3981
1186.6441	1197.7402	1247.0845
1331.0540	1410.6132	1426.2857
1450.3635	1500.7098	1581.2264
2964.5309	2968.9091	3177.4124
3177.8341	3195.4765	3198.0232

i6

C	-1.047827	0.872138	0.000004
C	0.227745	1.337151	-0.000019
C	-1.370645	-0.605834	-0.000006
C	-0.120866	-1.391379	0.000047
C	1.145926	-0.934528	-0.000055
C	1.352834	0.469791	0.000016
H	1.994371	-1.611693	0.000094
H	-1.993163	-0.857925	-0.872789
H	-1.993316	-0.857994	0.872634
H	2.357908	0.873224	0.000037
H	-1.885803	1.561421	0.000086
H	0.396997	2.408934	0.000023

Frequencies:

186.7376	399.3764	525.0064
551.6531	591.3049	659.7279
758.5138	879.7596	892.8371
927.4139	934.1290	979.6649
979.8340	995.2931	1102.4542
1176.5135	1187.4359	1271.3896
1323.0414	1355.5696	1420.8395
1450.2282	1547.8125	1606.7033
2975.5938	2988.0560	3175.9045
3178.3189	3195.7514	3214.8560

i7

C	-0.000000	1.204274	-0.759000
C	0.000000	1.204274	0.759000
C	0.000000	0.000000	-1.438272
C	0.000000	-1.204274	-0.759000
C	-0.000000	0.000000	1.438272
C	-0.000000	-1.204274	0.759000
H	-0.000001	2.149057	-1.286211
H	0.000001	2.149057	1.286211
H	0.000000	0.000000	-2.523444
H	0.000001	-2.149057	-1.286211
H	-0.000001	-2.149057	1.286211
H	-0.000000	0.000000	2.523444

Frequencies:

114.3673	298.7709	323.3570
346.2751	546.3424	598.9551
599.9177	629.3132	630.3703
632.1071	791.5792	921.3505
952.4113	959.7814	1003.0580
1075.3903	1166.1039	1172.1251
1307.1085	1358.9032	1402.4328
1443.2078	1501.2314	1531.0902
3182.9518	3184.4941	3211.3401
3221.6996	3224.3468	3234.8425

i8

C	0.567161	-0.760978	-0.420313
C	-0.801807	-1.162136	0.006499
C	-1.503617	0.000004	0.226711
C	-0.801804	1.162137	0.006497
C	0.567167	0.760975	-0.420313
C	1.398541	-0.000000	0.599129
H	2.472305	-0.000008	0.450238
H	1.067618	0.000003	1.631287
H	-1.138156	2.178788	0.146648
H	1.091276	1.326452	-1.182041
H	1.091275	-1.326460	-1.182033
H	-1.138169	-2.178784	0.146647

Frequencies:

358.2772	375.6113	497.8309
680.0716	687.2839	694.2936
774.3711	797.2567	807.1473
888.8123	950.9476	970.2199
1025.9272	1052.0709	1075.6427
1087.2107	1103.8813	1184.4714
1189.4704	1289.4243	1316.8783
1329.0763	1413.2249	1481.2037
3137.3453	3177.2005	3185.2037
3235.8142	3244.3622	3249.0809

Transition States:

i1 – i2

C	0.866519	-0.839775	-0.189713
C	0.813112	0.806574	-0.247638
C	-0.689285	1.005730	-0.299363
C	-1.357195	-0.052481	0.521837
C	-0.550676	-0.978328	-0.307374
C	1.377616	0.124755	0.872753
H	1.530168	-1.375840	-0.858930
H	1.406505	1.263092	-1.041680
H	-1.176365	1.519537	-1.117081
H	-2.430094	-0.130864	0.372142
H	-1.078571	-0.038376	1.579271
H	-1.012183	-1.636398	-1.036733

Frequencies:

-914.5645	323.5848	388.8827
400.8307	488.7013	563.8725
645.6518	783.5183	808.5595
871.7515	912.1498	951.0967
978.0328	999.0400	1066.6974
1114.3932	1149.7161	1175.4635
1217.6716	1275.0481	1292.8898
1353.7957	1392.2946	1471.1749
3058.3876	3103.9836	3176.2601
3181.9250	3199.8622	3230.7137

i1 – i3

C	-1.144777	0.106470	0.521763
C	1.220993	-0.676720	0.097982
C	-0.240971	1.175755	0.033568
C	-0.233605	-1.092681	-0.030231
C	1.110776	0.822034	0.006548
C	-1.105375	-0.240993	-0.850655
H	-1.834968	0.041556	1.354824
H	1.827194	-1.092445	-0.715468
H	1.655738	-1.034280	1.040821
H	-0.626343	2.165222	-0.176254
H	-0.554415	-2.101277	0.211659
H	1.890550	1.458031	-0.389437

Frequencies:

-663.9299	316.9567	429.9047
601.0278	661.1147	736.0920
780.2902	870.5700	875.6670
925.6523	931.5726	963.7929
975.1800	1000.4509	1062.7749
1101.5402	1151.3592	1187.4769
1246.5793	1297.0433	1323.9356
1409.6513	1431.1871	1468.3981
3019.6143	3060.7478	3176.4349
3183.2147	3217.1598	3234.0476

i2 – i4

C	-1.362625	-0.036465	0.145088
C	-0.518664	-1.261923	-0.059378
C	0.938602	-0.880207	-0.187201
H	-0.860883	-1.818051	-0.940761
H	-0.593223	-1.953122	0.790390
C	-0.753081	1.153987	-0.039886
C	0.675199	1.141498	-0.168127
H	1.186950	1.791933	-0.873025
C	1.428657	0.137033	0.597572
H	1.560059	-1.484205	-0.857267
H	-2.430089	-0.139091	0.298124
H	-1.311344	2.078999	-0.145870

Frequencies:

-825.9883	248.0237	381.1877
502.8102	563.2271	689.9822
710.0520	759.8277	894.9698
900.1394	913.7157	951.5040
993.1767	1011.1764	1117.1046
1141.8276	1159.2250	1189.8325
1251.4542	1322.1305	1396.5918
1439.4314	1456.6011	1593.7964
3030.6676	3060.5319	3068.8305
3158.5065	3179.8135	3213.3080

i4 – i5

C	-0.049620	1.349247	-0.009914
C	-1.264544	0.587377	-0.038196
C	-1.273703	-0.771207	0.014077
C	0.011950	-1.433094	0.021568
C	1.210208	-0.842227	-0.037016
C	1.274056	0.601907	-0.007999
H	0.678053	1.112183	1.026413
H	2.179716	1.142169	-0.246778
H	2.133154	-1.409133	-0.106536
H	-0.040797	2.406158	-0.236170
H	-2.202300	1.130283	-0.104317
H	-2.197903	-1.333680	0.012268

Frequencies:

-2657.0301	257.1922	371.1517
533.3160	561.9355	593.3409
605.2707	715.5030	767.3484
852.3638	874.8809	944.3328
967.3568	969.4553	998.9405
1118.2046	1160.9838	1223.5027
1276.2029	1322.6280	1353.6782
1426.5374	1516.3962	1615.5663
2209.6012	3180.8043	3182.1446
3218.0638	3221.5588	3232.9983

i4 – i6

C	-0.123196	1.344803	-0.029495
C	-1.268497	0.616584	0.005971
C	-1.216227	-0.854305	0.008671
C	-0.006998	-1.417973	-0.045332
C	1.255175	-0.790375	-0.012203
C	1.177422	0.746098	0.000555
H	1.382231	-0.011324	1.019687
H	2.073073	1.301794	-0.241658
H	2.182609	-1.263441	-0.302844
H	-0.176405	2.426851	-0.085712
H	-2.234130	1.107766	0.009945
H	-2.133452	-1.430636	0.031584

Frequencies:

-2476.2171	290.9511	404.9235
519.7048	556.8597	587.9453
603.6540	724.2782	759.8019
822.0883	861.7933	946.9655
955.3183	966.8301	1011.9954
1106.9996	1155.0199	1200.3031
1260.3830	1307.8727	1350.5125
1429.6993	1573.7810	1585.2398

i4 – p1

C	-0.115463	1.296110	-0.094357
C	1.160358	0.765448	-0.004515
C	1.348562	-0.621470	0.058205
C	0.217041	-1.399665	0.000652
C	-1.067324	-0.946413	-0.091502
C	-1.246054	0.457249	-0.072522
H	-2.224634	0.869774	-0.293141
H	-1.748393	0.690117	1.670453
H	-1.920906	-1.611906	-0.143958
H	-0.253514	2.369340	-0.147144
H	2.022549	1.423450	0.008028
H	2.342175	-1.048323	0.130002

Frequencies:

-1012.0531	287.7895	386.0415
437.4194	491.5477	599.7650
618.4950	670.6312	760.4791
858.3997	895.9293	987.1109
997.4460	1010.6861	1044.6432
1057.5203	1072.1765	1173.2715
1181.9429	1300.2550	1316.0007
1459.1034	1483.1318	1577.7239
1641.4314	3183.4572	3189.0493
3204.1825	3205.1478	3216.2573

i5 – i8

C	-0.699327	0.945525	-0.219834
C	0.639793	1.269361	-0.010839
C	1.456193	0.125482	0.268131
C	0.950732	-1.082691	-0.009608
C	-0.469207	-0.982884	-0.413390
C	-1.347871	-0.228993	0.485212
H	-2.411781	-0.301522	0.274875
H	-1.125968	-0.305755	1.550819
H	1.474071	-2.029225	0.039787
H	-0.841710	-1.436615	-1.326132
H	-1.327660	1.566633	-0.849726
H	1.051165	2.231682	-0.287658

Frequencies:

-761.0257	355.2797	405.9408
498.1160	597.1175	636.3001
704.6225	741.7528	794.9662
842.7629	921.5248	956.3217
1036.1876	1054.1326	1099.5522
1166.4591	1183.4584	1200.7113
1236.7816	1342.2012	1384.6393
1423.5625	1486.9385	1566.9274
3078.6465	3167.8792	3180.5621
3190.4837	3212.3870	3216.4327

i5 – p1

C	1.225171	-0.810184	0.009042
C	-1.225171	-0.810182	0.009042
C	-1.218498	0.576318	-0.095650
C	0.000001	1.281443	-0.086143
C	1.218498	0.576317	-0.095650
C	-0.000001	-1.434655	0.070412
H	2.156620	-1.364405	0.029302
H	-2.156622	-1.364402	0.029302
H	-2.154193	1.120834	-0.154328
H	0.000003	1.870807	1.691359
H	0.000001	2.341994	-0.307629
H	2.154194	1.120831	-0.154329

Frequencies:

-859.7375	297.3930	370.1077
423.5729	474.5402	600.4912
617.3180	703.3495	765.6025
816.3251	939.3749	979.7921
988.7396	1007.3900	1041.6972
1047.6868	1083.7987	1174.2592
1182.4784	1313.8747	1319.7601
1467.2692	1473.4685	1583.8675
1622.6940	3187.2954	3191.7312
3201.4143	3206.7930	3215.4072

i6 – i7

C	-1.178435	0.736482	-0.007836
C	0.021010	1.357708	0.027422
C	-1.300507	-0.709518	-0.042977
C	0.009034	-1.414874	-0.017215
C	1.259210	-0.754827	-0.039546
C	1.280639	0.606945	-0.010362
H	-2.094805	1.317486	-0.030333
H	0.062878	2.439955	0.059156
H	-2.191789	-1.210015	-0.397899
H	-0.723233	-1.289405	1.013220
H	2.178506	-1.330076	-0.071496
H	2.222729	1.140560	-0.029561

Frequencies:

-2885.1379	239.2781	337.4153
502.1367	555.9490	586.4964
627.7157	694.6189	785.3960
864.4080	934.6701	942.2622
958.6629	972.5642	990.2999
1045.2635	1158.2485	1187.4237
1240.6130	1299.1768	1363.8160
1440.8292	1507.7103	1617.4790
1440.8292	1507.7103	1617.4790
2216.2734	3180.3187	3186.6619

i6 – p1

C	1.045150	0.844377	-0.089967
C	-0.250092	1.322215	0.008173
C	1.291576	-0.548745	-0.090516
C	0.168980	-1.361970	-0.112184
C	-1.128734	-0.936256	-0.012262
C	-1.335562	0.445140	0.058953
H	-1.963786	-1.627458	0.001986
H	1.823554	-0.783306	1.699827
H	2.280025	-0.933731	-0.312833
H	-2.344914	0.833587	0.139110
H	1.882810	1.530990	-0.137954
H	-0.425594	2.391351	0.036682

Frequencies:

-848.0113	279.3374	373.0154
436.7726	483.3078	600.5985
617.6826	696.3895	737.4627
850.8931	937.8565	983.2267
998.6380	1014.5742	1015.3563
1046.9692	1071.9639	1176.2837
1183.3497	1300.0957	1323.3350
1460.7411	1472.2991	1584.3197
1635.7788	3185.4514	3191.1240
1635.7788	3185.4514	3191.1240
3199.7460	3204.8971	3216.0066

i7 – p1

C	-1.380135	-0.297809	0.326968
C	-1.057469	1.050114	0.147718
C	-0.425676	-1.283023	0.094479
C	0.858582	-0.942270	-0.318143
C	0.223313	1.326243	-0.259910
C	1.204724	0.398890	-0.504181
H	-2.379123	-0.572438	0.648516
H	-1.790185	1.829290	0.324754
H	-0.685040	-2.325825	0.236135
H	1.596639	-1.716906	-0.497064
H	2.201177	0.680319	-0.825380
H	4.516493	0.592696	3.191445

Frequencies:

-1133.9665	343.1611	385.2780
453.5941	492.9997	595.0651
624.4315	689.0175	739.3443
806.0896	907.3279	983.5110
984.5152	1009.4540	1021.8893
1040.2649	1091.8480	1178.2287
1183.2835	1306.9754	1310.6852
1462.5555	1464.1065	1593.6896
1615.6292	3184.8497	3190.9652
3204.6278	3207.6527	3216.5542

Product

p1 (C_6H_5)

C	-1.318480	-0.000000	0.000000
C	-0.629408	-1.208727	0.000000
C	-0.629408	1.208727	-0.000000
C	0.768043	1.221500	-0.000000
C	1.393311	0.000000	-0.000000
C	0.768043	-1.221500	0.000000
H	-2.402291	-0.000000	0.000000
H	-1.174711	-2.146572	0.000000
H	-1.174711	2.146572	-0.000000
H	1.319551	2.154848	-0.000000
H	1.319551	-2.154848	0.000000

Frequencies:

404.1763	429.8854	605.1739
623.4599	683.3133	731.2778
831.3365	908.5620	986.6279
993.0134	1013.5753	1031.1240
1058.4503	1085.1109	1182.4015
1184.9440	1310.4487	1326.8842
1474.4928	1485.6091	1610.2864
1662.7411	3181.6185	3187.6658
3199.6036	3202.8844	3213.9747