

Supporting Information for

Exotic Reaction Dynamics in the Gas-Phase Preparation of Anthracene (C₁₄H₁₀) via Spiroaromatic Radical Transients in the Indenyl–Cyclopentadienyl Radical–Radical Reaction

Chao He,¹ Ralf I. Kaiser,^{1*} Wenchao Lu,^{2†} Musahid Ahmed,^{2*} Yahaira Reyes,³ Stanislaw F. Wnuk,³ Alexander M. Mebel^{3*}

Affiliations

¹ Department of Chemistry, University of Hawai‘i at Manoa, Honolulu, HI 96822, USA

² Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

³ Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, USA

†present address: at CSIRO, Environment, Waite Campus, Urrbrae, South Australia 5064, Australia

Corresponding to: ralfk@hawaii.edu; mahmed@lbl.gov; mebela@fiu.edu

This PDF file includes:

Discussion of PIE Curves in Figure S1
Figures S1 to S2
Table S1

Discussion of PIE Curves in Figure S1

The experimental PIE curve of $m/z = 180$ is remarkably different with that of $m/z = 178$ suggests that the signal at $m/z = 180$ can be attributed to 1-(cyclopenta-2,4-dien-1-yl)-1H-indene intermediate ($C_{14}H_{12}$, **i1**) and 2-(cyclopenta-2,4-dien-1-yl)-2H-indene ($C_{14}H_{12}$, **i10**), which are the initial complexes via a recombination of both radical reactants with the radical centers located at the C1 carbon atom and the C2 carbon atom of 1-indenyl ($C_9H_7^\bullet$), respectively. The PIEs of $m/z = 178$, 152, 142, 130, 129, and 128 are superimposable revealing that the signals at $m/z = 178$, 152, 142, 130, 129, and 128 are originated from the same species. The overall shape of the PIE curve of $m/z = 178$ (Figure 3) can be reproduced via the contribution of the PIE curves of phenanthrene ($C_{14}H_{10}$, **p1**), anthracene ($C_{14}H_{10}$, **p2**), and benzofulvalene ($C_{14}H_{10}$, **p3**) with the branching ratios of the ion counts of 19.3 %, 8.4 %, and 72.3 % respectively. Therefore, the $m/z = 152$, 142, 130, 129, and 128 should be the fragments of $m/z = 178$ with molecular formulae as $C_{12}H_8$, $C_{11}H_{10}$, $C_{10}H_{10}$, $^{13}CC_9H_8$, $C_{10}H_8$, respectively.

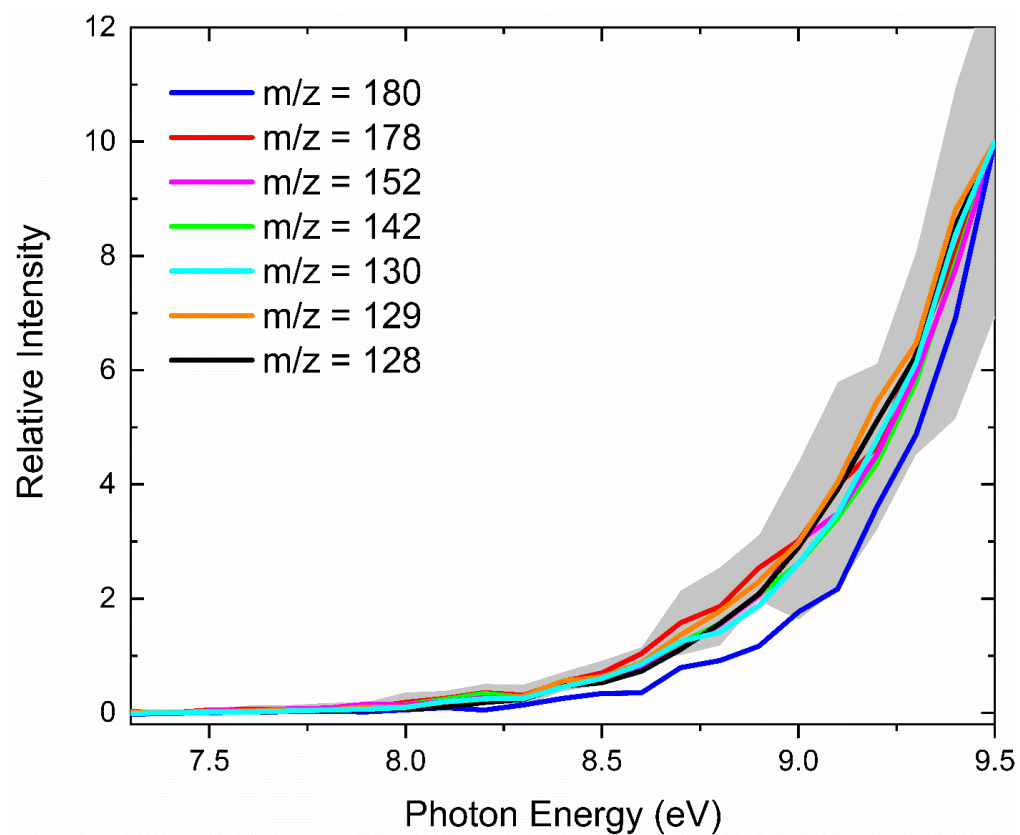


Figure. S1. Photoionization efficiency (PIE) curves for products ($m/z = 128 - 180$) in the reaction of the indenyl with cyclopentadienyl at a reactor temperature of 1473 ± 10 K.

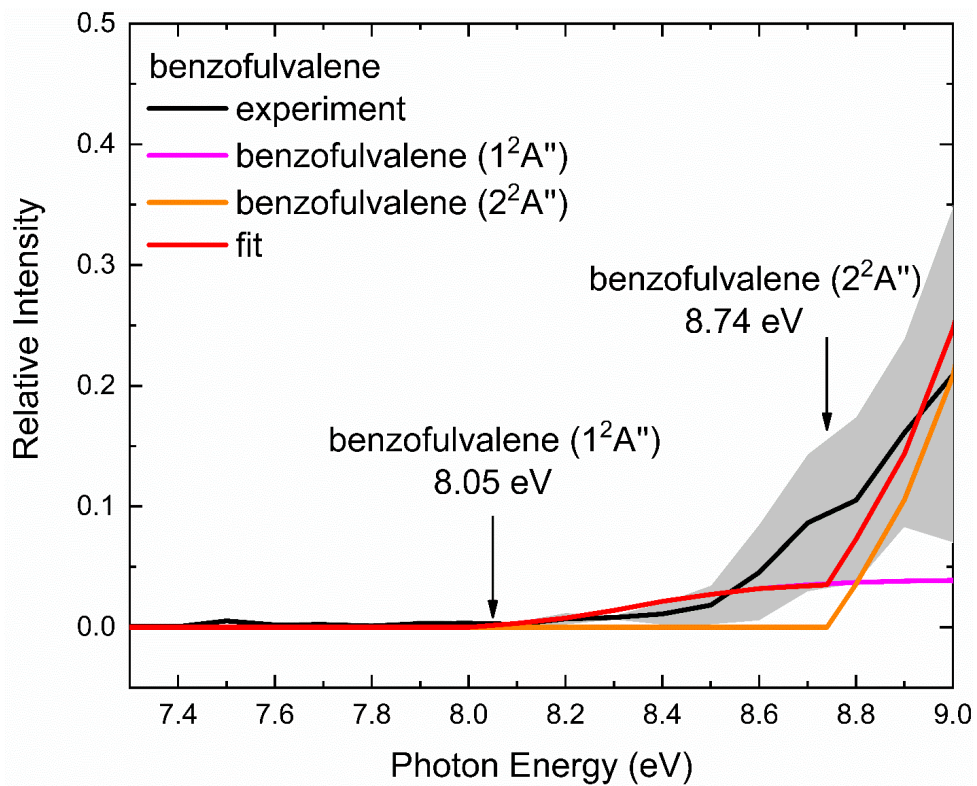


Figure. S2. Experimental PIE curve along with the fits for benzofulvalene in the reaction of the indenyl ($C_9H_7\bullet$) with cyclopentadienyl ($c-C_5H_5\bullet$) derived from experimental PIE of $m/z = 178$ in Figure 3(a).

Table S1. Optimized Cartesian Coordinates (Å) and vibrational frequencies (cm⁻¹) for the new calculated pathways that involved in the indenyl (C₉H₇•) plus cyclopentadienyl (c-C₅H₅•) reaction.

i10

C	-4.3529017758	1.6712823541	1.0276414489
C	-4.3311421494	0.2995002184	1.2734743489
C	-3.1820313528	-0.4647266200	1.0022704158
C	-2.0637008804	0.1719174536	0.4830740952
C	-2.0856540637	1.5784764621	0.2308702648
C	-3.2252083221	2.3248699975	0.5020035105
C	-0.7466413965	-0.3077364099	0.0993569420
C	0.0054840170	0.7674046168	-0.3693236020
C	-0.7877021507	1.9342622970	-0.3006404008
C	2.9606570772	2.4865913683	-0.9546233318
C	2.4711944921	2.2337956954	-2.3189927130
C	1.5825312238	1.2206866290	-2.2911287477
C	1.4262775030	0.7237896147	-0.8709339193
C	2.3672684417	1.6260109613	-0.1036308064
H	-5.2490928308	2.2404836213	1.2440968207
H	-5.2112482157	-0.1854672096	1.6790645070
H	-3.1769220233	-1.5315180762	1.1977805582
H	-3.2496712714	3.3926006517	0.3133862543
H	-0.4069904487	-1.3332364716	0.1670416414
H	-0.4695476489	2.9246324283	-0.5980740810
H	3.6838152450	3.2478252193	-0.6929379422
H	2.7858235974	2.7840780349	-3.1959861845
H	1.0369877837	0.8023423727	-3.1253082829
H	1.7862915898	-0.3127687352	-0.8080000404
H	2.5049645595	1.5604795263	0.9665262443

Frequencies

47.4690	72.8705	92.0973
165.4676	205.5562	259.2320
284.2812	371.8087	426.3174
450.1341	505.3664	543.9225
565.3039	577.6886	649.7052
657.6886	697.1722	713.4731
721.9827	740.1427	758.6479
812.7595	824.5664	827.1406
830.1935	855.9920	897.1871
909.1296	931.1740	939.5321
946.6000	951.5748	952.5353
984.9551	1010.4253	1032.3304
1046.1622	1069.4096	1112.5213
1118.6056	1143.4738	1152.9619
1179.5043	1186.9799	1199.4270
1248.1895	1259.6125	1284.5264
1309.5896	1326.0225	1394.9585
1400.2334	1407.7793	1452.2569
1544.4733	1552.7341	1579.6343
1607.5740	1631.9087	1686.4013
2999.5757	3018.1832	3181.0476
3188.4466	3201.0066	3209.8892
3210.1983	3221.3986	3222.3533
3236.3931	3236.8481	3248.2445

C	3.7341470000	-1.0959780000	-0.0000890000
C	4.0101850000	0.2702200000	0.0000830000
C	2.9703170000	1.2171760000	0.0000950000
C	1.6575370000	0.7675620000	-0.0000850000
C	1.3741220000	-0.6332140000	-0.0002710000
C	2.4078640000	-1.5608860000	-0.0002240000
C	0.3794910000	1.4593350000	0.0002450000
C	-0.6443260000	0.5143040000	0.0001590000
C	-0.0659540000	-0.7744560000	-0.0002110000
C	-3.8368220000	-0.6252150000	0.7354760000
C	-3.8369120000	-0.6244820000	-0.7359120000
C	-2.8548060000	0.1852510000	-1.1794090000
C	-2.1262900000	0.7898960000	0.0003990000
C	-2.8546470000	0.1840560000	1.1796690000
H	4.5509770000	-1.8078700000	-0.0001100000
H	5.0398060000	0.6081000000	0.0001870000
H	3.1974170000	2.2777040000	0.0003160000
H	2.2009200000	-2.6254980000	-0.0003340000
H	0.2463470000	2.5335170000	0.0003470000
H	-0.6157800000	-1.7062360000	-0.0004540000
H	-4.5244720000	-1.1920940000	1.3492340000
H	-4.5246110000	-1.1907830000	-1.3501540000
H	-2.5880230000	0.3927410000	-2.2061800000
H	-2.2782180000	1.8784460000	0.0009780000
H	-2.5877950000	0.3905660000	2.2066230000

Frequencies

28.7761	74.7745	78.4813
186.1272	222.6712	238.5816
343.3064	363.4853	412.4607
437.4924	530.1904	541.8002
575.1638	597.5930	601.6182
638.7695	681.3962	721.5443
739.9993	769.5919	771.5263
790.3277	817.7535	837.8551
846.6857	863.3253	889.5179
913.2564	922.6605	934.8553
942.0817	947.9358	994.4597
1018.6987	1033.5282	1036.8328
1101.5793	1112.2160	1122.4277
1147.7199	1171.9386	1184.7451
1212.0902	1226.8253	1228.4569
1247.4122	1312.7445	1324.0202
1351.5471	1403.1556	1430.2621
1492.8713	1497.0878	1543.2855
1554.2989	1630.1676	1632.9523
1664.7690	3029.0412	3182.6401
3188.3200	3199.1308	3212.0213
3212.4841	3221.1648	3222.1878
3230.7693	3241.4428	3247.3273

C	-0.2328060000	1.4664180000	-0.0002850000
C	-1.4187670000	0.7955570000	-0.0001120000
C	-2.7912560000	1.2412230000	0.0001170000
C	0.8270860000	0.4735820000	-0.0000560000
C	0.2102090000	-0.8467390000	-0.0005610000
C	-1.1361350000	-0.6583180000	-0.0002070000
C	2.2098390000	0.8263100000	0.7402930000
C	2.2100170000	0.8265290000	-0.7398630000
C	3.0106750000	-0.3322160000	-1.1416000000
C	3.4499030000	-0.9984250000	0.0000780000
C	3.0104430000	-0.3325310000	1.1418530000
C	-3.7788850000	0.3231840000	0.0002170000
C	-2.2425630000	-1.5879710000	-0.0000490000
C	-3.5022260000	-1.1100760000	0.0001350000
H	-0.0773790000	2.5366740000	-0.0002710000
H	-3.0129770000	2.3028510000	0.0001530000
H	0.7439300000	-1.7842870000	-0.0007960000
H	2.1336250000	1.7207210000	1.3411600000
H	2.1339360000	1.7211080000	-1.3404970000
H	3.1607920000	-0.6434460000	-2.1650100000
H	4.0114930000	-1.9230120000	0.0000060000
H	3.1603520000	-0.6440540000	2.1652040000
H	-4.8153790000	0.6415340000	0.0003160000
H	-2.0469970000	-2.6548300000	-0.0001810000
H	-4.3445960000	-1.7924100000	0.0001620000

Frequencies

59.5343	99.0504	127.8713
220.8148	252.9421	267.9030
294.2767	369.0893	445.3539
464.2946	525.8007	550.3344
577.7250	605.0188	608.9597
621.3333	673.5622	723.0281
741.4060	749.2783	750.8317
756.9707	803.8998	830.8700
844.4637	853.2833	881.2171
901.5266	915.0227	939.0646
946.9904	968.3917	977.1807
979.9593	982.7964	1049.8584
1054.9509	1086.2166	1086.8028
1124.9595	1154.0626	1177.4251
1194.4296	1228.8966	1281.1537
1294.1200	1299.8097	1335.0631
1342.1733	1399.1768	1407.1682
1421.2572	1448.8436	1486.4582
1549.3634	1656.1685	1682.1454
1786.8503	3176.8215	3183.6610
3198.0128	3208.0789	3223.5155
3223.9077	3226.6410	3233.1989
3246.2259	3255.3121	3257.8453

C	-0.0128640000	1.1851100000	0.0003120000
C	1.2742390000	0.7397360000	0.0001070000
C	2.5319560000	1.4426380000	-0.0000200000
C	-0.9619750000	-0.0000060000	0.0001290000
C	-0.0128580000	-1.1851190000	0.0003120000
C	1.2742420000	-0.7397380000	0.0001070000
C	-1.7995530000	-0.0000050000	-1.2572220000
C	-1.7998800000	-0.0000050000	1.2572520000
C	-3.1597490000	0.0000020000	1.2259540000
C	-3.8729550000	0.0000070000	-0.0002640000
C	-3.1594300000	0.0000020000	-1.2262960000
C	3.6868790000	0.7256010000	-0.0001480000
C	2.5319640000	-1.4426340000	-0.0000200000
C	3.6868830000	-0.7255910000	-0.0001480000
H	-0.3633870000	2.2079140000	0.0004040000
H	2.5447200000	2.5265540000	0.0000120000
H	-0.3633760000	-2.2079250000	0.0004040000
H	-1.2546850000	-0.0000080000	-2.1941170000
H	-1.2552580000	-0.0000080000	2.1942910000
H	-3.7119110000	0.0000040000	2.1594390000
H	-4.9549340000	0.0000120000	-0.0004060000
H	-3.7113480000	0.0000040000	-2.1599260000
H	4.6420290000	1.2380980000	-0.0002200000
H	2.5447320000	-2.5265490000	0.0000120000
H	4.6420350000	-1.2380840000	-0.0002200000

Frequencies

50.2507	63.6085	121.7063
204.4178	282.8893	287.7485
303.9589	435.4240	435.8509
439.3231	509.1929	527.0266
569.5045	570.3810	596.6163
597.4887	663.9652	664.3304
668.5000	727.7580	736.8133
776.1970	778.3854	789.2806
835.2385	835.8423	877.9899
909.1151	950.3552	952.2796
952.7561	955.1405	955.8957
985.2156	992.0696	1050.7521
1066.7174	1103.0517	1119.7784
1154.9182	1180.2907	1181.5050
1202.3053	1239.4715	1252.8064
1255.1259	1320.2088	1385.7011
1393.3700	1398.0448	1442.6238
1449.8129	1540.7483	1552.7835
1573.4409	1602.2803	1618.7529
1680.9618	3180.2454	3182.4637
3182.9793	3190.6078	3203.0063
3203.1677	3203.8236	3211.2128
3222.0670	3233.5249	3236.0369

C	-3.3262277450	0.5551924400	1.4249945550
C	-3.1966411700	-0.8715885320	1.2049740710
C	-1.9844284790	-1.4890724180	1.1980567030
C	-0.8004476910	-0.7010044390	1.4174393700
C	-0.9325494640	0.7534518750	1.6417326680
C	-2.2422619320	1.3497761490	1.6358277040
C	0.5204800700	-1.0422104700	1.4672901470
C	1.3403421820	0.1998203240	1.7036146110
C	0.3085600260	1.2910733210	1.8271306940
C	4.0185076810	0.8295042420	-0.8002646120
C	2.8280795670	0.8516766050	-1.6460351070
C	1.7459094310	0.6300123740	-0.8468844120
C	2.2342237190	0.4624245740	0.5277140060
C	3.6291633580	0.5903637000	0.5207948170
H	-4.3201639960	0.9874380870	1.4162067700
H	-4.0988476330	-1.4493212550	1.0404395560
H	-1.8999067120	-2.5565938510	1.0302014430
H	-2.3515392130	2.4160760760	1.7970244500
H	0.9529796810	-2.0216669160	1.3188272780
H	1.9446928460	0.1141110190	2.6152750120
H	0.5577265140	2.3302237430	1.9899627170
H	5.0321372080	0.9754380310	-1.1488658080
H	2.8261869080	1.0161291720	-2.7135201060
H	0.7064584790	0.5800845660	-1.1361105940
H	4.2759493660	0.5163245860	1.3822760690

Frequencies

43.1358	54.0619	89.9056
186.5347	210.0032	276.3016
315.4590	373.8837	425.3018
453.9151	504.5695	527.5710
566.4818	577.2471	628.2897
646.5222	662.1008	702.4512
708.2102	725.7851	744.8475
747.8965	768.1325	833.6636
834.9254	841.4818	855.8310
873.8043	904.1636	909.2790
947.4464	955.4773	955.5394
984.3437	988.9029	1032.9460
1039.8987	1098.9429	1125.4179
1137.4610	1180.3736	1185.9205
1215.6728	1219.1996	1248.5228
1266.4801	1288.4903	1320.3957
1396.5184	1400.1883	1428.1298
1445.6751	1458.1635	1527.4305
1570.4933	1574.9078	1600.8824
1683.6044	3050.6333	3184.1847
3191.7019	3203.9228	3212.1010
3223.1233	3236.5150	3237.1081
3239.5087	3248.1831	3257.8715

C	-0.2502830000	1.7305010000	-0.5415780000
C	-1.2686520000	0.7334120000	-0.1900170000
C	-2.5816590000	1.2026420000	-0.0059450000
C	1.0607650000	1.6936670000	-0.2675310000
C	0.2534410000	-1.3007130000	-0.3653790000
C	-1.0344930000	-0.6674620000	-0.1312310000
C	1.4852290000	-0.7642420000	-0.1163520000
C	1.7121140000	0.5935470000	0.5332060000
C	3.2142150000	0.6790080000	0.6144660000
C	3.7710030000	-0.4578910000	0.1046840000
C	2.7545010000	-1.3481760000	-0.3442630000
C	-3.6410940000	0.3490190000	0.2557910000
C	-2.1367410000	-1.5181980000	0.0963310000
C	-3.4146450000	-1.0290660000	0.3035250000
H	-0.6292120000	2.6004290000	-1.0712010000
H	-2.7588180000	2.2707210000	-0.0760800000
H	1.6955060000	2.4993440000	-0.6219940000
H	0.2162670000	-2.3228690000	-0.7327180000
H	1.2719170000	0.5800960000	1.5417780000
H	3.7442450000	1.5269880000	1.0260560000
H	4.8324580000	-0.6598680000	0.0423720000
H	2.9179160000	-2.3171170000	-0.7963090000
H	-4.6372590000	0.7478030000	0.4057530000
H	-1.9615410000	-2.5885260000	0.1167450000
H	-4.2336800000	-1.7132790000	0.4913540000

Frequencies

69.3591	110.8408	167.5340
211.7012	283.4906	306.3893
334.8310	356.5572	411.7736
480.8948	513.0400	533.8949
552.5551	583.6211	637.6505
679.0623	690.2855	703.5380
727.7663	737.8296	761.5748
767.2063	807.9272	835.6637
841.4838	871.6666	889.4124
903.7353	948.2891	950.4128
956.6871	985.3891	1008.6592
1039.4469	1071.3671	1079.5429
1123.5692	1139.7970	1190.4178
1194.0072	1207.5989	1230.3298
1246.5369	1253.0992	1271.9765
1299.6481	1317.3206	1366.4974
1369.7379	1405.5454	1428.1931
1472.9966	1524.6054	1532.5345
1582.6458	1621.7817	1662.1814
1720.6530	2995.8765	3155.8773
3159.6661	3178.4721	3182.9492
3185.2983	3198.4911	3213.1714
3213.8564	3228.1991	3241.1492

p4

C	0.0000000000	0.7261030000	-3.9220630000
C	0.0000000000	-0.7261030000	-3.9220630000
C	0.0000000000	-1.4435860000	-2.7659860000
C	0.0000000000	1.4435860000	-2.7659860000
C	0.0000000000	-0.7445390000	-1.5110550000
C	0.0000000000	0.7445390000	-1.5110550000
C	0.0000000000	-1.1832730000	-0.2138950000
C	0.0000000000	1.1832730000	-0.2138950000
C	0.0000000000	0.0000000000	0.6473350000
C	0.0000000000	-0.7398550000	4.1742090000
C	0.0000000000	0.7398550000	4.1742090000
C	0.0000000000	1.1789080000	2.8925720000
C	0.0000000000	-1.1789080000	2.8925720000
C	0.0000000000	0.0000000000	2.0156360000
H	0.0000000000	1.2384720000	-4.8772800000
H	0.0000000000	-1.2384720000	-4.8772800000
H	0.0000000000	-2.5277480000	-2.7805400000
H	0.0000000000	2.5277480000	-2.7805400000
H	0.0000000000	-2.2063090000	0.1305160000
H	0.0000000000	2.2063090000	0.1305160000
H	0.0000000000	-1.3536870000	5.0643700000
H	0.0000000000	1.3536870000	5.0643700000
H	0.0000000000	2.2024590000	2.5513390000
H	0.0000000000	-2.2024590000	2.5513390000

Frequencies

54.4047	85.9201	111.9775
157.5934	234.5855	250.6005
325.8507	333.4892	433.5758
486.2851	507.8863	530.2657
562.1342	587.7580	595.0440
618.9527	620.1359	671.3566
707.3670	710.5321	745.5939
758.2607	778.2182	800.3875
820.7191	850.2868	901.1879
907.4126	907.5533	919.0220
946.3012	946.3856	974.6405
984.3657	1024.4538	1098.6680
1114.1889	1120.5295	1154.3250
1179.4409	1193.7745	1218.3082
1247.9959	1286.4276	1324.7804
1382.3415	1391.3744	1395.7879
1446.0814	1522.6776	1546.3621
1569.4267	1589.0373	1598.6610
1668.3241	1670.8479	3181.5599
3188.1060	3200.7553	3210.1315
3225.2604	3236.0553	3248.0839
3249.8507	3261.7573	3265.3275

Transition state **i11** to **i12**

C	-0.2271270000	1.4804070000	0.0741690000
C	-1.4250980000	0.7979560000	0.0317170000
C	-2.7864070000	1.2360350000	-0.0450390000
C	0.8163080000	0.5002150000	0.1565620000
C	0.2137110000	-0.8261940000	0.1496370000
C	-1.1409120000	-0.6473790000	0.0760460000
C	2.2526180000	0.8628110000	0.6570760000
C	2.2320190000	0.7954030000	-0.8187830000
C	2.9452260000	-0.3890450000	-1.1958690000
C	3.4176340000	-1.0247830000	-0.0295650000
C	3.0478490000	-0.3010670000	1.0851450000
C	-3.7776840000	0.3094130000	-0.0786670000
C	-2.2330980000	-1.5818340000	0.0336850000
C	-3.5009040000	-1.1129940000	-0.0393690000
H	-0.0795700000	2.5513980000	0.0676990000
H	-3.0135740000	2.2960640000	-0.0754290000
H	0.7543040000	-1.7586710000	0.1863010000
H	2.2791690000	1.7996650000	1.1980160000
H	2.0166080000	1.6263720000	-1.4703830000
H	3.0464920000	-0.7522310000	-2.2079650000
H	3.9504580000	-1.9660770000	-0.0128260000
H	3.2215590000	-0.5698340000	2.1167540000
H	-4.8123700000	0.6285380000	-0.1369220000
H	-2.0307470000	-2.6470720000	0.0642190000
H	-4.3371360000	-1.8018210000	-0.0699320000

Frequencies

337.8677i	74.2635	99.3088
134.4293	225.6141	257.4395
265.3785	357.6876	434.0188
463.2941	505.1868	530.0483
557.3667	583.3949	600.2749
643.6633	661.7560	731.0699
737.2714	742.1395	760.1492
764.8534	808.3397	822.8544
833.4355	840.6649	864.7415
905.4975	910.3133	939.4756
944.3446	965.7923	967.4039
987.9072	991.6879	1038.3925
1063.3496	1076.8778	1089.8759
1122.9334	1149.5081	1170.2405
1192.8383	1217.1640	1265.2574
1293.1487	1314.9380	1338.5975
1357.6677	1394.6305	1403.5870
1429.3481	1435.2909	1502.0851
1508.5123	1613.8984	1627.5943
1730.2738	3176.9862	3183.5276
3197.3442	3206.0152	3208.2024
3224.6652	3228.8736	3246.2213
3253.9811	3261.3191	3269.0684

Transition state **i12** to **i13**

C	0.2052430000	1.4482800000	-0.0862410000
C	1.3940630000	0.7832240000	-0.0428280000
C	2.7558550000	1.2486970000	-0.0205950000
C	-0.8994520000	0.4464790000	-0.0865690000
C	-0.2177230000	-0.8850820000	-0.0532000000
C	1.1279920000	-0.6736370000	-0.0178310000
C	-2.0576080000	0.6978050000	-0.9784750000
C	-1.9764240000	0.7122190000	1.0029380000
C	-3.0275820000	-0.1610160000	1.1984160000
C	-3.4932690000	-0.8980530000	0.0428950000
C	-3.0515840000	-0.3611620000	-1.1249500000
C	3.7642030000	0.3364990000	0.0270340000
C	2.2387880000	-1.5879380000	0.0366350000
C	3.5047560000	-1.0901310000	0.0566710000
H	0.0476080000	2.5183550000	-0.1110880000
H	2.9644220000	2.3124930000	-0.0413530000
H	-0.7410960000	-1.8290840000	-0.0437820000
H	-2.1156810000	1.6358330000	-1.5185740000
H	-1.7772280000	1.5435940000	1.6663910000
H	-3.5924350000	-0.1439480000	2.1233780000
H	-4.1973230000	-1.7166670000	0.1076840000
H	-3.3957080000	-0.6669050000	-2.1058200000
H	4.7951960000	0.6710470000	0.0443850000
H	2.0568550000	-2.6565210000	0.0591640000
H	4.3518390000	-1.7653050000	0.0962030000

Frequencies

789.0873i	62.8319	111.2880
127.2503	213.7666	280.4092
291.3942	395.3361	411.2680
445.2777	473.7219	510.3110
535.5687	563.3379	578.7575
616.4505	644.2248	653.3970
670.3957	713.6818	724.1351
733.2379	749.7632	787.8266
817.6947	828.3718	840.1798
865.4222	900.4268	907.3396
911.0773	931.9508	947.9766
949.3954	985.1869	1024.5238
1046.7172	1117.4687	1129.3474
1146.7218	1148.6535	1182.0553
1182.4094	1216.1249	1268.5844
1298.1537	1309.8061	1373.9963
1392.2792	1398.2723	1406.3799
1452.5714	1459.8464	1573.7076
1589.1532	1597.9637	1604.6673
1678.383	3180.6897	3187.7893
3191.3208	3192.3213	3200.3286
3202.0675	3209.5022	3213.2377
3223.4663	3229.6591	3253.5292

Transition state **i13** to **i9**

C	0.1054280000	1.4268270000	0.2627480000
C	1.3161330000	0.7951430000	0.1527120000
C	2.6522220000	1.2218920000	0.4741500000
C	-0.9727760000	0.4866260000	-0.1506140000
C	-0.2321450000	-0.7396240000	-0.6234730000
C	1.1155270000	-0.5549900000	-0.3734330000
C	-2.1483590000	0.9758590000	-0.9306630000
C	-3.3746320000	0.4276850000	-0.7772100000
C	-3.6399890000	-0.5697430000	0.2195800000
C	-2.6542620000	-0.9109040000	1.1387710000
C	-1.3667200000	-0.4052970000	1.0399510000
C	3.6842200000	0.3675660000	0.2647790000
C	2.2351380000	-1.4226230000	-0.5542330000
C	3.4800500000	-0.9631930000	-0.2577500000
H	-0.0868080000	2.4161900000	0.6534240000
H	2.8196500000	2.2158490000	0.8728770000
H	-0.7277290000	-1.5862150000	-1.0731120000
H	-1.9718100000	1.7723160000	-1.6429500000
H	-4.1969200000	0.7826060000	-1.3886120000
H	-4.6383150000	-0.9767090000	0.3147770000
H	-2.9007060000	-1.5403760000	1.9869260000
H	-0.6225610000	-0.5478020000	1.8110010000
H	4.6966760000	0.6777600000	0.4974080000
H	2.0850670000	-2.4251250000	-0.9388790000
H	4.3444450000	-1.5998330000	-0.4047530000

Frequencies

524.0779i	83.1531	116.4486
145.4119	259.1835	277.8865
320.7936	364.7402	433.4986
449.896	478.0695	530.3837
564.6818	578.7981	592.6968
612.7313	663.7112	684.6862
695.2546	734.5557	746.9085
761.5303	791.5352	797.9874
848.5468	855.9276	885.5911
891.3817	914.7240	929.7485
966.9889	968.1235	978.0548
982.0227	992.8255	1001.2820
1076.2402	1107.8148	1150.1366
1157.6695	1175.8633	1182.9099
1189.7177	1223.3760	1249.7995
1265.6675	1307.4367	1361.6070
1400.4758	1403.9066	1439.3845
1454.5078	1484.7686	1512.7702
1591.0015	1612.2290	1648.7226
1711.2868	3182.9591	3183.1979
3186.6718	3190.5479	3203.3252
3209.5939	3212.6282	3218.8411
3231.4065	3236.7776	3259.1360

Transition state **i4** to **i8**

C	-0.8375115629	-0.5038234586	-0.2267660440
C	-0.3889257781	2.0229637650	-0.3070190362
C	0.9601402227	1.7093029619	-0.2221093317
C	-1.4525617904	0.8274230256	-0.2096817024
C	-1.4515478429	1.6901957730	1.0219854132
C	-2.6418289317	2.4609472881	0.9960544621
C	-3.3675419323	2.1493469666	-0.1747142557
C	-2.7095483788	1.1752024824	-0.8959946929
C	2.8109602907	0.1518778821	0.2945549154
C	1.4328726634	0.4132463229	0.0841680342
C	0.5099161743	-0.7094754756	0.0287809950
C	1.0539548914	-2.0294899323	0.1683384929
C	2.3893022695	-2.2311854941	0.3887630246
C	3.2831008794	-1.1290493716	0.4572988304
H	-1.4825063453	-1.3507179556	-0.4317197132
H	-0.7202594806	2.9318802599	-0.7908103285
H	1.6840313634	2.4770490466	-0.4775879514
H	-0.8534727941	1.4705556560	1.8925870397
H	-2.9157670886	3.1992947400	1.7369077596
H	-4.2867262059	2.6338670593	-0.4782051133
H	-3.0008614917	0.7679626270	-1.8542662157
H	3.4969118651	0.9925351111	0.3227680998
H	0.3740463140	-2.8731892569	0.1121354526
H	2.7731658297	-3.2383294005	0.5077416133
H	4.3394118600	-1.3036636222	0.6262002520

Frequencies

88.5472	130.1951	
189.314	246.3157	325.0077
331.4079	357.6922	376.6567
447.3602	475.9483	511.6369
539.5203	575.4040	602.4052
634.8602	660.8829	705.5458
722.3089	742.6838	757.4657
764.8774	772.8124	803.0871
825.249	849.4416	851.3923
866.2792	910.8408	944.8458
949.9177	956.4402	963.7818
979.8988	1037.2203	1071.2417
1084.414	1099.8778	1113.0133
1136.8371	1166.1699	1182.4262
1209.6709	1239.9719	1270.5535
1290.8794	1297.6499	1332.6053
1383.1896	1387.2714	1422.6890
1438.0353	1454.3168	1495.1347
1509.8698	1575.5711	1581.7095
1659.8017	3174.3254	3176.7353
3181.072	3193.3873	3195.9019
3208.8997	3214.8026	3216.4958
3231.748	3241.9490	3253.9029

Transition state **i8** to **i9**

C	0.4633649725	-1.2224009852	-0.0904859661
C	1.3085057047	-0.2622744578	0.3835114672
C	2.6872882904	-0.5527391757	0.7299876777
C	-0.9484997879	-0.9583626276	-0.3740664521
C	-0.3758129506	1.4748127341	0.0030382322
C	0.8794012246	1.1352318129	0.4640460018
C	-1.3248724110	0.5122185104	-0.3988418660
C	-1.8778899832	-0.7252532827	0.8210170090
C	-3.2676224705	-0.6050151239	0.6509614767
C	-3.6647116645	0.1387600303	-0.5033074619
C	-2.6210087098	0.8359684539	-1.0353580888
C	3.5211372617	0.4196977884	1.1564354534
C	1.8133154592	2.1251305679	0.9222165812
C	3.0809119711	1.7909175035	1.2622922981
H	0.8491578080	-2.2157260199	-0.2953404502
H	3.0248212850	-1.5806558297	0.6558541013
H	-1.4082464460	-1.5701056442	-1.1498937115
H	-0.6568852250	2.5220569583	-0.0613417790
H	-1.4114890259	-0.8046694202	1.7959629511
H	-3.9508508963	-0.8616951547	1.4508468330
H	-4.6863245990	0.2066789214	-0.8535663455
H	-2.6809669633	1.5280838498	-1.8654188415
H	4.5436985483	0.1772027384	1.4225235600
H	1.4740236458	3.1535440259	0.9883801844
H	3.7766409616	2.5454378265	1.6080161358

Frequencies

88.8398	113.8423	
190.7671	227.6246	307.2596
342.8225	364.4753	394.7001
443.7127	454.6252	520.2747
525.6000	556.1286	612.0558
634.9425	657.0434	678.5238
689.4363	697.7758	737.3511
750.8199	788.1712	834.8160
838.0984	854.9528	877.5730
900.9781	914.6398	919.1766
960.6230	981.6533	990.0722
999.5311	1041.8043	1055.4458
1103.9129	1122.5616	1138.6352
1153.9021	1179.5084	1190.3469
1217.4943	1242.7884	1297.6904
1310.6058	1326.7861	1342.6090
1379.5251	1402.6092	1430.5761
1437.9734	1469.4247	1491.3013
1555.3930	1624.3294	1662.2225
1728.7934	3102.9157	3174.0976
3179.6982	3180.9149	3185.0913
3189.3851	3201.2122	3206.2237
3212.2174	3214.6845	3231.1305

Transition state **i14** to **i3**

C	-3.193945341	0.719785024	1.132305257
C	-3.093349816	-0.683670977	0.80917826
C	-1.910948279	-1.35000539	0.904690703
C	-0.75739992	-0.644192515	1.356563184
C	-0.852766319	0.777675052	1.687681643
C	-2.122564429	1.438588142	1.551683961
C	0.544108339	-1.064626357	1.576727282
C	1.36214723	0.1284904	1.944143313
C	0.380857864	1.241107545	2.062568356
H	-4.158965841	1.202118066	1.02674827
H	-3.984740354	-1.202685842	0.477722923
H	-1.83756163	-2.401231373	0.651123125
H	-2.210672417	2.49342792	1.784167506
H	0.944204549	-2.061562524	1.472663736
H	2.093838798	0.02206166	2.743905012
H	0.645481298	2.256756426	2.318894915
C	3.543753429	-0.368242338	-1.036833096
C	2.427132776	0.346549258	-1.642773576
C	1.49546185	0.600121117	-0.673909572
C	2.017634144	0.067581767	0.576321282
C	3.279164156	-0.550992748	0.302654161
H	4.433726386	-0.69057756	-1.560176719
H	2.356606254	0.620866411	-2.685719289
H	0.545791478	1.099042056	-0.787304679
H	3.914931796	-1.024523219	1.036753042

Frequencies

326.3162i	64.5410	88.4168
105.4432	195.7097	241.5061
318.6054	369.0215	416.7845
470.356	510.0496	544.7870
554.2937	582.5715	594.1439
663.6502	686.7721	693.9810
723.6496	744.6109	749.8366
763.8657	805.1233	830.1684
845.9083	851.9593	860.1242
872.7908	897.3280	916.8333
971.3288	979.4793	982.3173
999.762	1020.3373	1038.4423
1079.7516	1098.5194	1103.8683
1151.7792	1159.9249	1196.5961
1225.7062	1236.2661	1253.4380
1272.7398	1311.2520	1319.5574
1357.6939	1404.7097	1406.7717
1426.0449	1465.0106	1480.6606
1563.3932	1588.1934	1609.1536
1703.4058	3128.8970	3186.6428
3194.8155	3206.7841	3215.4251
3219.7302	3233.7638	3244.0020
3245.1769	3260.3913	3262.7094