Dissociation of the Anthracene Radical Cation: A Comparative Look at iPEPICO and Collision-Induced Dissociation Mass Spectrometry Results

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Supplementary Information

Complete Reference 43

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Figure S1: illustrative TOF fittings for iPEPICO TOF focussing on the asymmetric $[M-C_2H_2]^+$ peak from the dissociation of the anthracene radical cation. It is demonstrating the appearance and eventual formation of the Gaussian shape. Photon energies for each spectrum is listed



Table S1: Vibrational frequencies (cm⁻¹) of neutral anthracene, anthracene radical cation and initial transition state estimates for fragmentation products. Frequencies in brackets indicate the frequency removed for each transition state, which were subsequently scaled during the fitting exercise according to the procedure outlined in the methods section. Bottom three values for M, M⁺⁺ and M-H⁺ are the rotational constants used for fitting, values are in GHz.

$C_{14}H_{10}$	$C_{14}H_{10}^{+}$	TS	TS	TS	$C_{14}H_{9}^{+}$	TS
(M)	(M ⁺⁻)	(M-H)⁺	$(M-C_2H_2)^{+}_{\sigma=6}$	$(M-C_2H_2)^{+}_{\sigma=1}$	(M-H) ⁺	[(M-H)-H] ^{+·}
95	90	(3335)	(1411)	(1411)	90	(3229)
127	126	67	70	47	121	90
242	228	94	98	67	227	121
246	239	171	178	121	238	227
280	284	179	186	127	276	238
405	393	213	222	151	357	276
407	402	393	393	393	382	357
411	407	402	402	402	391	382
501	459	407	407	407	423	391
507	479	459	459	459	433	423
525	501	479	479	479	476	433
551	532	501	501	501	514	476
611	581	532	532	532	539	514
635	629	581	581	581	584	539
661	644	629	629	629	608	584
682	688	644	644	644	629	608
777	753	688	688	688	708	629
781	769	753	753	753	739	708
795	793	769	769	769	755	739
806	803	793	793	793	765	755
807	812	803	803	803	772	765
851	866	812	812	812	782	772
885	915	866	866	866	817	782
907	944	915	915	915	832	817
950	947	944	944	944	881	832
950	957	947	947	947	919	881
960	977	957	957	957	924	919
1026	990	977	977	977	936	924
1032	1044	990	990	990	962	936
1051	1051	1044	1044	1044	996	962
1052	1079	1051	1051	1051	1025	996
1063	1080	1079	1079	1079	1049	1025
1069	1094	1080	1080	1080	1085	1049
1173	1095	1094	1094	1094	1098	1085
1186	1167	1095	1095	1095	1157	1098
1222	1204	1167	1167	1167	1182	1157
1238	1228	1204	1204	1204	1200	1182

1239	1249	1228	1228	1228	1217	1200
1261	1254	1249	1249	1249	1233	1217
1342	1258	1254	1254	1254	1272	1233
1343	1332	1258	1258	1258	1299	1272
1353	1355	1332	1332	1332	1310	1299
1397	1361	1355	1355	1355	1337	1310
1415	1368	1361	1361	1361	1382	1337
1476	1411	1368	1368	1368	1413	1382
1490	1470	1411	1470	1470	1417	1413
1503	1483	1470	1483	1483	1441	1417
1550	1492	1483	1492	1492	1481	1441
1553	1552	1492	1552	1552	1498	1481
1587	1555	1552	1555	1555	1536	1498
1661	1599	1555	1599	1599	1593	1536
1682	1607	1599	1607	1607	1600	1593
1705	1650	1607	1650	1650	1643	1600
1758	1652	1650	1652	1652	1711	1643
1762	1685	1652	1685	1685	3188	1711
3276	1694	1685	1694	1694	3200	3188
3277	3302	1694	3302	3302	3203	3200
3281	3304	3302	3304	3304	3205	3203
3282	3309	3304	3309	3309	3207	3205
3285	3310	3309	3310	3310	3212	3207
3287	3312	3310	3312	3312	3218	3212
3300	3313	3312	3313	3313	3228	3218
3300	3325	3313	3325	3325	3229	3228
3312	3325	3325	3325	3325		
3312	3335	3325	3335	3335		
3325	3335	3335	3335	3335		
2.172	2.179				2.155	
0.456	0.456				0.464	
0.377	0.377				0.382	



Figure S2. CBS-QB3 reaction energy path to C_2H_2 loss from anthracene and phenantrene cations. Although the isomerization path from anthracene to phenantrene probably lies below the C2H2-loss transition states, it is unlikely to channel the reactive flux along a higher lying and tighter path to biphenylene. At yet higher energies, a new path may open up to yield the most stable product, acenaphthalene.