Harmonic vibrational frequencies of circumanthracene ($C_{40}H_{16}$) in the four charge states -1, 0, +1 and +2. All calculations were performed at the B3LYP/4-31g level of theory.

Numb. of the mode	Anion		Neutral		Cation		Dication	
	Freq. (cm^{-1})	Int. (km mol^{-1})	Freq. (cm^{-1})	Int. (km mol^{-1})	Freq. (cm^{-1})	Int. (km mol^{-1})	Freq. (cm^{-1})	Int. (km mol^{-1})
1	44	0.2	42	0.5	43	1.0	41	1.8
2	46	0.0	46	0.0	47	0.0	48	0.0
3	100	0.0	99	0.0	99	0.0	97	0.0
4	103	0.9	102	3.0	100	6.1	97	10.4
5	110	0.0	109	0.0	110	0.0	110	0.0
6	148	0.0	148	0.0	146	0.0	143	0.0
7	164	0.0	162	0.1	163	1.2	162	3.3
8	197	0.0	199	0.0	198	0.0	195	0.0
9	206	8.2	207	4.3	206	2.4	207	0.2
10	240	0.0	245	0.0	245	3.6	241	3.1
11	251	3.3	246	3.8	245	0.0	244	0.0
12	260	0.0	260	0.0	257	0.0	252	0.0
13	270	0.0	271	0.0	271	0.0	270	0.0
14	276	0.0	278	0.0	277	0.0	275	0.0
15	280	0.0	284	0.0	286	0.0	285	0.0
16	294	0.0	293	0.0	290	0.0	286	0.0
17	344	0.4	338	0.1	334	0.1	325	0.2
18	352	0.0	364	0.0	361	0.0	353	0.0
19	360	0.0	366	0.0	369	0.0	373	0.0
20	371	0.0	370	0.0	373	0.0	374	0.0
21	388	0.0	387	0.0	388	1.1	385	3.8
22	389	1.2	389	0.5	389	0.0	389	0.0
23	402	8.9	401	9.3	401	9.4	400	8.8
24	403	0.0	411	0.0	411	0.0	407	0.0
25	410	0.0	413	0.0	415	0.0	420	0.0
26	425	1.2	427	0.0	428	0.1	427	0.5
27	427	0.0	428	0.1	428	0.0	427	0.0
28	481	0.0	481	0.0	474	0.0	464	0.0
29	487	0.0	487	0.0	480	0.0	473	0.0
30	488	10.3	489	0.9	489	0.0	486	0.6
31	496	0.0	496	0.0	495	0.6	488	0.0
32	498	0.0	503	0.0	497	0.0	496	0.0
33	502	0.0	505	0.0	504	0.0	503	0.0
34	531	0.0	533	0.0	532	0.0	527	0.0
35	532	1.8	533	2.3	533	1.4	528	22.8
36	539	7.0	540	11.4	534	16.1	532	0.0
37	565	0.0	565	0.0	565	0.0	563	0.0
38	566	0.0	567	0.0	568	0.0	566	0.2
39	567	0.2	568	0.0	569	0.0	569	22.6
40	569	18.6	570	0.1	570	5.2	571	0.0
41	571	17.0	572	18.2	573	19.6	572	20.2
42	589	0.0	596	0.0	592	0.0	589	0.0
43	604	0.0	612	0.0	611	0.0	610	0.0
44	619	0.0	618	0.0	619	0.0	619	0.0
45	630	0.0	636	0.0	634	0.0	631	0.0
46	636	0.0	638	0.0	635	0.0	634	0.0
47	637	0.0	640	0.0	636	0.0	635	0.0
48	650	0.0	649	0.0	651	0.0	651	0.0
49	658	0.0	657	0.1	657	0.6	656	2.5
50	685	0.0	684	0.0	683	0.0	681	0.0
51	695	7.6	700	0.5	697	3.3	694	12.4
52	706	0.0	711	0.0	708	3.0	704	3.0

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Table 1 - continued from previous page

Numb. of the mode	Anion Freq. (cm^{-1})	Anion Int. (km mol^{-1})	Neutral Freq. (cm^{-1})	Neutral Int. (km mol^{-1})	Cation Freq. (cm^{-1})	Cation Int. (km mol^{-1})	Dication Freq. (cm^{-1})	Dication Int. (km mol^{-1})
53	707	2.9	713	2.6	712	0.0	713	0.0
54	715	3.0	714	1.7	715	1.0	713	0.1
55	737	0.0	748	0.0	747	0.0	745	0.0
56	747	0.0	754	2.9	752	6.6	749	6.4
57	749	2.8	760	0.0	755	0.0	754	0.0
58	752	0.0	763	0.0	760	2.0	756	3.7
59	754	1.0	764	2.2	765	0.0	764	0.0
60	760	0.0	768	0.0	770	2.6	771	6.2
61	763	0.0	769	0.1	772	0.0	774	0.0
62	764	0.0	774	0.0	779	0.0	776	0.0
63	767	0.3	781	0.0	783	0.0	778	0.0
64	768	0.0	783	5.5	786	0.0	796	0.0
65	778	0.0	789	0.0	791	6.4	798	5.8
66	790	0.0	805	0.0	805	0.0	803	0.0
67	799	0.0	805	0.0	815	0.0	811	0.0
68	799	0.0	812	0.0	817	0.0	830	0.0
69	799	0.0	815	0.0	824	0.0	836	0.0
70	815	0.0	839	0.0	853	0.0	868	0.0
71	819	47.8	849	102.0	862	121.9	873	149.5
72	823	0.0	863	0.0	881	0.0	900	0.0
73	835	0.0	869	0.0	886	0.0	909	0.0
74	855	195.8	898	0.0	899	0.0	913	0.0
75	856	0.0	905	133.8	917	1.6	916	1.9
76	895	0.0	905	0.0	925	0.0	933	49.5
77	916	0.6	916	1.9	925	114.0	956	2.2
78	925	0.0	939	2.5	938	5.1	958	0.0
79	925	0.0	952	0.0	954	0.2	958	86.8
80	933	1.2	953	0.0	974	0.0	977	0.0
81	940	0.0	954	3.6	975	0.0	989	0.0
82	940	0.2	972	0.0	977	0.0	992	0.0
83	945	0.0	973	0.2	985	0.0	998	0.0
84	946	0.0	974	0.0	986	0.0	999	0.1
85	949	0.7	977	0.0	995	0.0	1011	0.0
86	972	0.0	978	0.0	995	0.0	1011	0.0
87	1016	1.0	1017	1.5	1024	13.6	1026	44.1
88	1044	0.0	1048	0.0	1054	0.0	1057	0.0
89	1095	0.0	1100	0.0	1104	0.0	1100	0.0
90	1098	0.0	1104	0.0	1108	0.0	1112	0.0
91	1103	2.5	1104	9.3	1113	4.1	1115	1.3
92	1135	0.0	1141	0.0	1146	0.0	1148	0.0
93	1141	4.3	1147	6.9	1155	18.2	1161	55.0
94	1148	17.6	1154	1.3	1161	1.9	1163	7.5
95	1154	0.0	1156	0.0	1164	0.0	1168	0.0
96	1158	1.4	1157	8.7	1166	2.4	1171	6.6
97	1177	0.0	1176	0.1	1187	32.2	1176	0.0
98	1178	1.3	1190	0.0	1188	0.0	1194	43.3
99	1202	0.0	1205	0.0	1209	0.0	1213	0.0
100	1209	44.1	1209	0.2	1213	57.8	1215	0.0
101	1212	0.0	1209	0.0	1217	0.0	1216	123.7
102	1214	13.5	1224	0.0	1219	6.6	1222	72.2
103	1217	0.0	1225	2.5	1220	0.0	1223	0.0
104	1228	0.4	1236	0.0	1234	0.0	1232	10.7
105	1239	0.0	1252	0.0	1246	319.1	1248	0.0
106	1244	69.5	1263	8.9	1248	0.0	1250	255.5

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Numb. of the mode	Anion Freq. (cm^{-1})	Anion Int. (km mol^{-1})	Neutral Freq. (cm^{-1})	Neutral Int. (km mol^{-1})	Cation Freq. (cm^{-1})	Cation Int. (km mol^{-1})	Dication Freq. (cm^{-1})	Dication Int. (km mol^{-1})
107	1270	0.0	1278	0.0	1279	0.0	1281	0.0
108	1277	25.2	1284	17.1	1288	14.1	1291	5.3
109	1298	0.0	1299	12.8	1302	0.0	1302	0.0
110	1302	826.9	1313	0.0	1323	282.5	1333	113.4
111	1316	40.3	1322	0.0	1329	13.8	1333	6.0
112	1316	0.0	1324	13.9	1334	0.0	1345	0.0
113	1333	18.8	1338	1.3	1342	152.2	1348	895.2
114	1344	17.6	1349	0.0	1356	86.2	1362	0.0
115	1345	0.0	1362	2.0	1359	0.0	1366	0.0
116	1358	0.0	1367	0.0	1371	0.0	1366	97.2
117	1359	2.1	1374	3.5	1371	26.6	1375	0.0
118	1361	0.0	1379	0.0	1377	0.0	1380	24.7
119	1370	23.9	1380	0.2	1382	2.9	1383	0.5
120	1383	0.0	1389	0.0	1392	0.0	1387	348.0
121	1385	42.5	1391	0.0	1400	28.5	1402	0.0
122	1386	0.0	1397	6.6	1401	0.0	1403	0.0
123	1386	0.0	1413	1.5	1402	8.0	1406	9.4
124	1413	0.0	1421	0.3	1424	0.9	1425	0.0
125	1415	0.2	1423	0.0	1429	40.5	1427	2.4
126	1418	112.1	1434	0.0	1430	0.0	1431	88.4
127	1422	0.0	1435	0.0	1431	0.0	1435	0.0
128	1431	0.0	1435	10.9	1438	0.0	1435	0.0
129	1436	0.0	1442	0.0	1442	0.0	1446	0.0
130	1453	60.2	1463	0.3	1468	1.2	1461	28.8
131	1461	1.3	1473	0.0	1472	0.0	1472	11.7
132	1464	0.0	1476	1.2	1473	16.1	1479	0.0
133	1468	22.1	1482	5.4	1480	16.0	1485	0.0
134	1485	6.2	1504	10.8	1489	0.7	1486	53.0
135	1494	0.0	1511	0.0	1500	0.0	1492	276.1
136	1512	0.0	1521	0.0	1518	0.0	1508	0.0
137	1517	0.0	1539	1.9	1523	32.0	1521	37.5
138	1535	0.0	1552	0.0	1536	0.0	1530	0.0
139	1544	0.0	1569	0.7	1551	25.7	1541	183.1
140	1550	0.5	1573	0.0	1558	0.0	1541	0.0
141	1569	249.7	1588	15.2	1568	176.2	1567	350.6
142	1575	0.0	1593	0.0	1585	0.0	1574	0.0
143	1583	0.4	1594	9.6	1586	0.0	1579	408.5
144	1586	16.0	1602	0.0	1586	9.8	1581	17.7
145	1587	0.0	1607	0.0	1587	94.9	1584	0.0
146	1591	0.0	1615	21.8	1590	0.0	1599	0.0
147	3017	0.0	3043	0.0	3060	0.0	3065	0.1
148	3017	5.6	3043	7.0	3060	2.0	3065	0.0
149	3019	45.3	3043	0.2	3063	5.9	3067	0.0
150	3019	0.0	3044	0.0	3063	0.0	3067	0.0
151	3021	0.0	3044	0.0	3064	0.0	3077	0.0
152	3021	16.4	3045	0.2	3065	7.5	3077	0.0
153	3025	5.1	3045	24.7	3065	0.4	3077	0.1
154	3026	0.0	3046	0.0	3066	0.0	3077	0.0
155	3031	86.3	3048	36.8	3066	0.0	3078	0.0
156	3031	0.0	3048	0.0	3066	0.0	3078	0.3
157	3041	51.4	3063	4.1	3081	1.6	3091	0.2
158	3041	0.0	3063	0.0	3081	0.0	3091	0.0
159	3044	0.0	3065	0.0	3083	0.0	3092	0.0
160	3044	340.9	3065	157.1	3083	48.5	3092	2.1

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Numb. of the mode	Anion		Neutral		Cation		Dication	
	Freq. (cm^{-1})	**Int.** (km mol^{-1})	**Freq.** (cm^{-1})	**Int.** (km mol^{-1})	**Freq.** (cm^{-1})	**Int.** (km mol^{-1})	**Freq.** (cm^{-1})	**Int.** (km mol^{-1})
161	3045	422.6	3066	222.3	3084	103.2	3093	15.7
162	3046	0.0	3066	0.0	3084	0.0	3093	0.0