Harmonic vibrational frequencies of benzo[a]coronene ($C_{28}H_{14}$) 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	37	0.0	40	0.1	39	0.1	34	0.1
2	64	0.0	66	0.0	66	0.0	63	0.0
3	95	0.0	104	0.0	101	0.0	95	0.0
4	108	0.4	108	2.2	106	5.2	104	8.5
5	128	1.1	128	1.6	126	3.2	122	6.0
6	192	0.0	193	0.0	189	0.0	184	0.0
7	216	4.9	218	0.8	215	0.3	198	2.8
8	239	0.0	235	0.0	229	0.0	219	0.0
9	281	0.0	283	0.0	274	0.0	261	0.0
10	286	0.0	288	0.0	278	0.1	269	0.3
11	299	1.3	302	0.0	300	1.1	286	16.7
12	306	0.3	318	0.6	315	0.7	298	1.3
13	319	0.0	331	0.0	326	4.5	309	0.6
14	337	0.7	345	0.0	333	0.0	331	0.0
15	380	2.1	380	2.5	381	3.1	381	1.5
16	407	12.5	412	0.9	405	0.3	394	2.6
17	411	0.2	419	0.5	415	1.9	398	2.7
18	417	2.2	426	1.5	418	2.4	417	3.7
19	464	5.9	466	0.0	457	0.0	443	3.4
20	468	0.8	469	6.6	458	4.5	444	0.0
21	470	0.0	473	0.1	467	0.1	462	0.2
22	492	8.0	495	0.1	494	0.0	464	0.0
23	495	0.0	498	0.8	494	1.8	489	1.0
24	499	0.0	518	0.0	495	0.0	493	2.0
25	537	1.5	542	5.8	522	6.8	499	9.1
26	546	0.0	547	0.0	541	0.0	534	0.0
27	548	7.0	553	0.3	551	1.0	550	1.7
28	550	0.5	567	5.0	567	7.8	568	10.1
29	596	22.8	600	1.8	598	3.4	593	24.2
30	600	0.0	607	0.8	603	0.6	598	0.1
31	611	0.0	625	0.0	623	0.0	617	0.0
32	634	4.6	648	0.0	639	0.0	635	0.0
33	642	0.0	653	0.3	650	0.0	646	0.1
34	651	0.1	660	6.5	661	8.1	661	8.8
35	666	0.5	669	3.5	666	0.7	662	2.9
36	681	3.4	682	0.3	681	0.2	679	0.0
37	717	0.0	728	0.0	719	0.0	704	0.0
38	727	0.0	735	1.3	733	0.5	723	8.0
39	729	0.7	748	2.3	741	21.7	733	48.4
40	729	64.3	750	0.0	745	26.6	735	21.6
41	734	30.9	750	51.4	753	0.0	754	0.0
42	735	0.9	761	10.7	765	13.7	754	21.7
43	758	1.0	778	7.3	767	38.4	770	0.0
44	768	0.0	785	1.1	783	0.0	771	43.6
45	768	0.2	799	0.0	790	0.0	795	44.7
46	787	4.5	806	0.2	805	7.7	798	1.3
47	788	0.0	806	0.0	818	0.0	831	0.0
48	798	5.6	819	11.6	830	10.4	841	3.2
49	806	0.0	841	0.0	851	1.0	843	12.1
50	817	124.7	855	2.2	857	0.0	873	0.0
51	832	0.0	856	125.2	873	139.2	887	0.0
52	844	7.9	858	0.0	873	0.0	889	150.0

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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	881	3.7	935	2.4	942	8.6	911	38.6
54	892	0.0	943	0.7	945	2.1	939	2.6
55	897	0.2	950	0.0	954	1.8	969	1.3
56	905	0.0	950	0.0	967	0.0	973	29.6
57	908	1.6	955	0.3	973	0.4	983	0.0
58	934	3.6	960	0.0	983	0.0	989	0.8
59	937	0.0	970	0.0	989	0.1	999	2.2
60	938	15.0	977	0.0	998	0.0	1002	0.0
61	939	0.0	984	0.0	1000	0.2	1009	0.3
62	988	0.1	995	0.2	1007	0.0	1015	0.0
63	1016	0.0	1026	0.1	1014	6.9	1025	0.0
64	1040	16.9	1042	4.8	1046	11.7	1042	72.9
65	1068	5.9	1072	0.0	1078	0.4	1044	31.4
66	1070	92.2	1104	0.1	1101	0.1	1082	0.4
67	1103	47.3	1148	3.9	1133	46.2	1092	1.2
68	1132	9.7	1153	2.0	1149	1.5	1144	7.6
69	1140	18.9	1164	0.0	1157	51.7	1148	0.3
70	1150	8.8	1168	0.4	1163	15.2	1158	3.8
71	1154	0.8	1182	1.8	1170	2.2	1163	101.8
72	1174	2.9	1185	0.1	1193	0.0	1193	0.1
73	1187	5.1	1192	0.0	1205	9.8	1199	7.3
74	1207	44.5	1220	0.9	1221	88.0	1226	22.1
75	1212	68.3	1224	1.2	1225	47.2	1228	3.7
76	1220	0.1	1227	0.6	1233	15.2	1232	147.0
77	1225	7.5	1239	2.0	1235	0.9	1244	23.4
78	1253	29.4	1240	1.3	1259	179.2	1262	1.2
79	1253	164.1	1263	13.7	1267	3.1	1273	6.1
80	1260	1.5	1299	0.9	1283	5.6	1286	190.3
81	1282	238.0	1302	6.9	1302	14.3	1295	339.3
82	1294	252.7	1319	5.7	1316	215.5	1329	99.6
83	1315	6.6	1333	17.0	1330	0.3	1331	39.1
84	1323	275.5	1336	1.0	1343	0.9	1336	311.9
85	1327	5.9	1356	0.1	1354	0.3	1353	14.4
86	1330	21.5	1379	0.1	1356	189.6	1367	0.0
87	1348	20.6	1381	0.7	1372	4.0	1368	45.4
88	1359	11.8	1386	0.1	1380	13.8	1374	15.3
89	1376	5.8	1400	1.1	1389	1.6	1379	6.8
90	1384	13.4	1413	0.6	1402	49.5	1406	54.1
91	1419	1.9	1428	4.8	1430	1.0	1426	1.8
92	1429	1.7	1430	0.0	1440	4.9	1447	41.2
93	1435	13.9	1446	6.0	1457	9.8	1451	11.8
94	1445	8.5	1462	1.4	1457	6.6	1461	55.6
95	1456	119.4	1473	9.5	1474	1.6	1470	12.4
96	1460	22.9	1489	2.1	1474	22.8	1472	5.4
97	1468	4.6	1491	7.5	1484	0.4	1484	125.2
98	1482	25.9	1523	0.0	1486	26.3	1488	46.3
99	1496	0.2	1533	1.4	1509	0.4	1491	56.2
100	1524	11.7	1537	0.3	1528	27.4	1535	105.0
101	1524	24.5	1569	0.0	1536	55.1	1540	191.1
102	1544	254.1	1594	4.3	1551	149.7	1541	236.6
103	1559	63.9	1597	0.4	1561	352.0	1554	201.2
104	1570	27.2	1600	0.5	1576	2.6	1562	347.3
105	1576	0.7	1603	6.5	1581	0.8	1575	11.1
106	1587	81.4	1607	9.2	1599	27.9	1610	35.2

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Table 1 - continued from previous page

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})
107	3007	4.0	3043	2.4	3069	0.2	3079	0.0
108	3012	53.8	3044	3.1	3070	0.2	3079	0.0
109	3013	0.3	3046	1.4	3071	0.0	3081	0.9
110	3021	3.2	3051	21.0	3073	7.4	3081	0.1
111	3024	0.9	3051	0.0	3073	0.1	3084	0.7
112	3024	39.7	3054	9.4	3079	0.9	3093	0.5
113	3033	73.3	3063	3.7	3086	0.0	3095	0.1
114	3038	165.9	3065	76.3	3087	14.5	3095	1.9
115	3039	198.3	3067	88.0	3088	28.1	3099	0.0
116	3042	62.9	3069	26.5	3091	6.6	3103	0.4
117	3056	31.8	3085	0.0	3102	0.5	3111	0.1
118	3059	0.0	3088	2.2	3106	8.0	3115	0.9
119	3078	108.8	3104	54.1	3123	16.0	3132	0.2
120	3082	58.3	3106	36.3	3124	15.3	3133	0.8