

Harmonic vibrational frequencies of benzo[a]anthracene (C₁₈H₁₂) 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	60	0.1	64	0.5	62	1.1	54	0.5
2	67	0.1	67	0.0	66	0.1	65	1.6
3	139	0.3	143	0.4	137	0.5	128	1.3
4	160	1.6	162	0.3	160	0.8	158	1.5
5	181	0.1	184	0.8	180	2.0	174	3.5
6	260	0.2	266	0.7	255	0.8	234	1.4
7	279	0.2	285	0.4	279	1.0	272	0.6
8	299	1.6	302	0.7	295	3.2	293	3.5
9	350	0.2	353	0.2	350	0.3	347	0.0
10	360	0.0	391	0.0	387	1.5	381	0.1
11	416	3.9	422	2.7	413	6.1	398	8.8
12	446	4.1	449	1.9	439	13.1	417	20.9
13	456	3.1	469	9.5	443	0.6	441	3.8
14	489	10.1	491	0.0	488	1.6	459	3.8
15	509	0.9	513	1.1	494	0.7	464	0.5
16	531	1.3	534	0.6	514	5.4	479	1.2
17	536	3.2	540	4.6	522	31.7	510	5.2
18	560	0.3	570	1.7	539	0.0	520	48.6
19	579	19.9	580	4.3	577	0.2	569	13.7
20	621	0.3	631	2.4	622	0.8	614	3.2
21	652	0.0	656	3.6	653	3.3	641	1.1
22	671	3.5	688	3.9	680	3.8	664	3.9
23	696	16.6	719	0.3	711	2.3	703	3.5
24	706	8.0	739	2.2	739	3.1	725	14.6
25	712	20.5	749	67.5	753	4.6	748	7.0
26	728	8.1	758	0.1	756	61.7	752	26.3
27	740	18.2	758	1.2	759	9.6	768	76.2
28	749	0.0	779	10.3	769	24.5	771	3.3
29	750	16.3	785	0.6	787	0.9	779	1.3
30	774	45.9	809	21.0	827	26.5	852	28.0
31	779	66.1	846	0.0	866	1.2	869	7.6
32	787	31.3	869	0.2	872	2.4	884	1.6
33	825	3.1	871	2.9	877	1.2	891	4.4
34	828	5.6	883	54.1	908	0.3	902	5.3
35	852	11.8	904	6.9	909	40.9	941	24.4
36	864	18.7	908	0.3	924	3.8	957	6.6
37	884	1.9	943	3.3	968	1.3	963	12.4
38	897	1.4	956	5.5	974	4.9	988	1.4
39	908	0.3	975	0.1	977	6.1	998	8.6
40	910	3.0	980	0.1	991	0.3	1011	0.2
41	937	0.0	987	0.0	1014	0.0	1015	21.8
42	966	2.3	989	0.0	1016	0.0	1018	35.1
43	1014	23.7	1008	1.8	1024	3.8	1032	0.7
44	1021	14.6	1038	3.1	1027	0.3	1036	0.7
45	1078	27.1	1099	0.3	1098	21.2	1084	57.7
46	1109	23.3	1135	1.5	1128	1.0	1115	26.4
47	1136	21.4	1157	1.7	1154	41.4	1131	75.1
48	1146	30.3	1168	1.4	1185	5.1	1170	18.5
49	1158	11.7	1178	0.0	1188	20.2	1194	29.9
50	1163	17.4	1184	2.8	1192	1.2	1198	19.4
51	1199	6.3	1204	0.9	1210	1.8	1202	50.4
52	1220	83.1	1223	2.3	1233	177.9	1238	150.9

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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})
53	1229	41.5	1242	7.6	1243	70.7	1257	23.5
54	1247	1.6	1266	1.0	1264	0.6	1267	12.5
55	1267	57.7	1289	2.4	1287	48.0	1286	386.1
56	1280	20.4	1299	1.2	1301	46.5	1305	21.2
57	1296	26.8	1317	1.0	1320	3.6	1318	17.3
58	1315	767.1	1339	4.2	1335	618.9	1339	391.8
59	1341	6.5	1353	2.3	1355	8.9	1369	14.1
60	1352	47.1	1381	0.0	1373	142.8	1390	37.9
61	1384	36.5	1416	1.2	1416	2.0	1411	26.0
62	1407	31.8	1419	0.9	1429	5.2	1426	15.2
63	1416	9.3	1443	0.3	1438	0.5	1435	27.1
64	1442	14.6	1457	5.9	1454	0.7	1445	16.1
65	1448	17.0	1480	3.5	1472	121.4	1474	69.6
66	1473	3.5	1495	18.8	1492	9.9	1493	120.6
67	1487	16.8	1540	2.2	1499	29.3	1507	27.7
68	1508	233.7	1546	0.0	1523	144.0	1512	0.3
69	1524	47.6	1583	0.4	1535	43.1	1529	371.1
70	1532	13.9	1599	1.2	1550	8.8	1541	127.8
71	1546	23.6	1612	1.1	1557	76.0	1550	35.8
72	1572	31.5	1618	3.1	1588	70.0	1591	231.7
73	2999	0.4	3040	4.8	3065	0.9	3068	2.0
74	3002	4.8	3043	2.1	3072	0.1	3080	0.2
75	3005	11.8	3044	10.2	3074	0.9	3082	1.9
76	3007	44.4	3046	3.6	3075	1.1	3085	0.0
77	3010	16.0	3048	1.8	3076	1.3	3087	0.7
78	3021	34.6	3056	9.0	3080	1.1	3088	0.4
79	3022	111.1	3063	15.5	3087	0.0	3091	7.3
80	3029	137.6	3064	59.6	3088	6.5	3092	2.9
81	3033	76.4	3065	19.3	3091	2.2	3098	4.3
82	3042	88.1	3075	34.1	3099	8.4	3107	1.0
83	3043	136.2	3079	55.4	3104	11.3	3112	8.6
84	3067	62.5	3088	29.2	3106	10.4	3113	2.1