

Harmonic vibrational frequencies of benzo[a]pyrene (C₂₀H₁₂) 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	56	0.0	59	0.3	59	0.8	55	1.3
2	78	0.0	84	0.0	81	0.2	75	1.1
3	151	0.5	152	0.7	152	1.1	149	1.7
4	176	0.0	182	0.1	178	0.2	169	0.5
5	210	2.9	209	5.1	200	9.3	191	14.0
6	214	1.8	212	0.9	210	0.3	208	0.0
7	268	0.0	280	0.0	273	0.2	262	0.4
8	303	0.5	301	0.0	302	0.4	296	3.0
9	328	0.2	330	0.1	329	0.4	327	0.3
10	371	0.5	379	0.1	375	0.2	370	0.5
11	373	0.7	387	0.1	385	0.0	379	0.0
12	454	4.4	457	0.9	445	2.7	425	3.6
13	455	2.0	458	2.7	453	2.2	448	2.7
14	479	0.1	481	0.4	480	1.3	451	1.3
15	489	1.2	501	0.5	482	2.3	462	0.0
16	509	0.5	515	4.0	490	1.1	477	0.8
17	515	5.1	515	0.7	513	2.4	509	0.8
18	522	8.6	525	1.1	525	0.9	510	1.2
19	526	1.0	535	3.7	525	3.8	524	16.7
20	560	0.2	562	0.0	548	3.5	538	9.6
21	566	3.2	569	0.9	564	2.1	560	4.6
22	602	14.3	609	0.1	608	4.6	604	19.0
23	636	1.0	641	4.5	638	0.1	631	4.3
24	652	0.2	672	0.3	664	2.5	653	4.3
25	682	7.8	689	11.8	679	9.3	666	6.2
26	696	5.6	700	1.2	699	0.3	693	1.2
27	703	16.5	742	14.9	739	15.3	723	34.0
28	712	10.8	750	13.0	757	57.1	753	10.8
29	733	45.3	759	47.5	759	3.0	765	20.0
30	746	4.0	760	0.6	764	6.9	777	27.8
31	752	1.4	800	0.0	804	1.0	807	1.6
32	768	4.2	813	4.9	812	4.6	808	30.1
33	796	29.9	815	0.2	826	0.0	844	0.4
34	805	1.0	835	43.4	849	58.2	848	11.7
35	808	6.4	847	0.1	851	1.4	865	71.4
36	813	44.8	852	17.7	874	12.2	885	2.7
37	830	19.4	890	1.6	889	1.4	896	5.2
38	842	17.4	892	24.7	916	24.9	956	13.5
39	876	4.0	903	11.0	934	1.8	970	2.0
40	881	8.8	946	2.9	969	2.8	980	30.4
41	897	0.0	963	0.5	982	7.1	991	2.6
42	906	0.9	972	0.9	983	0.3	1002	2.0
43	924	0.2	976	0.2	990	0.2	1009	0.9
44	929	0.2	982	0.4	1008	0.1	1016	14.0
45	969	2.0	987	0.2	1013	0.0	1032	0.1
46	1012	4.5	1019	1.6	1022	0.9	1036	0.6
47	1035	15.0	1035	2.0	1041	3.5	1038	27.0
48	1070	8.9	1078	1.4	1082	0.3	1080	2.8
49	1103	1.3	1109	0.1	1120	6.7	1114	18.2
50	1119	2.0	1122	0.4	1133	1.6	1140	3.9
51	1137	15.1	1157	1.1	1155	17.2	1146	54.7
52	1162	8.8	1167	1.3	1176	9.0	1168	5.7

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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})
53	1168	3.5	1180	0.9	1189	4.0	1196	2.3
54	1172	10.7	1189	7.3	1199	24.6	1203	49.6
55	1190	13.5	1202	2.9	1206	36.3	1208	115.5
56	1210	5.3	1226	0.2	1226	4.6	1225	18.1
57	1232	102.6	1245	0.6	1245	157.9	1238	180.1
58	1256	8.9	1252	3.6	1268	3.6	1269	32.1
59	1262	12.9	1275	5.3	1276	4.4	1272	60.0
60	1278	30.2	1311	1.1	1297	12.6	1297	26.0
61	1304	124.0	1324	0.4	1331	57.0	1334	98.2
62	1314	116.3	1340	4.2	1342	47.7	1352	81.0
63	1322	122.7	1354	0.4	1345	91.6	1360	215.1
64	1343	9.9	1365	0.6	1367	12.2	1376	0.2
65	1352	6.0	1402	4.9	1389	18.4	1377	21.1
66	1399	13.9	1416	1.1	1424	5.6	1424	19.4
67	1410	5.5	1420	3.2	1429	0.5	1434	19.2
68	1414	30.2	1429	1.4	1433	15.0	1437	0.3
69	1433	23.3	1454	2.6	1443	4.6	1453	2.6
70	1464	1.3	1468	1.5	1472	41.3	1466	192.7
71	1473	1.3	1488	5.9	1479	9.2	1491	94.7
72	1491	0.5	1509	3.7	1506	59.8	1494	84.5
73	1508	3.6	1551	2.0	1529	48.7	1521	94.9
74	1524	93.1	1566	3.0	1537	25.6	1526	7.7
75	1535	172.3	1587	4.3	1542	71.8	1537	181.1
76	1544	7.7	1591	2.3	1547	43.4	1545	163.4
77	1560	22.4	1604	3.6	1570	69.4	1563	219.8
78	1579	102.7	1619	2.9	1589	73.6	1592	134.0
79	3001	46.4	3041	2.1	3064	0.9	3066	0.9
80	3003	0.4	3044	2.8	3072	0.2	3079	0.6
81	3006	18.9	3046	2.1	3073	0.9	3082	0.3
82	3013	24.3	3047	8.5	3073	1.3	3083	1.8
83	3015	13.6	3049	3.3	3075	0.6	3083	1.8
84	3024	23.5	3055	17.8	3078	1.9	3084	2.0
85	3024	47.7	3057	20.6	3083	1.4	3091	2.4
86	3029	161.6	3065	48.0	3088	6.0	3095	4.2
87	3037	197.6	3073	48.9	3097	1.8	3105	0.0
88	3040	61.9	3075	42.4	3102	7.7	3111	5.6
89	3050	53.9	3082	20.7	3104	8.7	3113	4.2
90	3065	93.1	3097	40.0	3114	8.8	3120	0.5