

Harmonic vibrational frequencies of benzo[g,h,i]perylene (C₂₂H₁₂) 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	63	0.0	59	0.0	66	0.0	69	0.0
2	92	0.0	94	0.3	90	1.0	85	2.2
3	134	1.2	131	3.3	129	6.8	125	11.3
4	172	0.0	178	0.0	180	0.0	176	0.0
5	194	0.8	200	1.9	194	2.9	186	4.0
6	266	0.0	274	0.0	272	0.0	259	0.0
7	286	0.0	286	0.5	276	0.0	269	0.0
8	286	2.9	290	0.0	286	1.6	281	1.3
9	290	0.0	292	0.0	288	0.3	282	1.5
10	358	4.7	363	0.1	359	3.8	359	12.8
11	381	0.7	383	0.1	385	0.6	384	0.9
12	404	24.1	409	2.4	406	0.4	398	0.6
13	404	0.4	424	0.1	413	0.1	403	0.3
14	448	0.5	450	0.9	440	0.0	422	0.0
15	464	0.0	453	0.0	449	1.0	444	1.2
16	480	2.0	481	0.1	478	1.3	472	0.0
17	504	0.0	514	4.6	499	0.1	475	4.5
18	512	10.0	529	0.0	503	0.0	475	0.9
19	530	0.1	532	0.1	528	1.7	517	6.6
20	533	1.2	537	0.4	529	10.4	523	5.5
21	537	1.4	543	6.8	532	0.3	527	0.9
22	555	1.4	566	1.9	559	0.5	549	0.5
23	571	0.0	575	0.0	576	0.0	577	0.0
24	626	6.2	632	0.0	626	0.9	619	0.4
25	627	0.0	647	0.0	636	0.0	622	27.8
26	630	0.0	649	9.2	637	18.6	623	0.0
27	678	2.2	678	0.3	677	0.4	675	0.1
28	678	0.0	714	0.3	707	0.0	701	14.6
29	705	2.7	714	0.0	708	5.8	704	0.0
30	711	42.6	756	32.5	739	24.1	722	18.6
31	729	0.0	763	1.9	764	7.9	752	28.1
32	740	20.1	768	0.0	773	0.0	768	0.1
33	765	0.7	775	2.9	773	16.7	770	0.0
34	766	0.0	779	4.4	775	0.2	786	28.8
35	772	16.8	801	0.2	802	6.7	799	35.7
36	773	7.1	809	28.3	809	20.0	811	11.1
37	791	4.3	814	0.0	813	0.0	820	0.0
38	792	8.4	834	0.0	847	0.0	865	0.0
39	795	0.0	851	107.0	868	111.8	887	116.9
40	813	0.0	893	0.0	913	20.0	905	42.9
41	817	93.8	902	6.5	922	0.0	941	1.7
42	891	0.0	920	0.0	929	9.3	955	0.0
43	895	0.9	945	1.2	945	0.2	961	9.8
44	904	19.7	956	0.0	978	0.0	991	0.5
45	918	0.0	968	0.6	987	0.4	997	0.0
46	925	0.3	970	0.0	989	0.3	1006	0.4
47	933	0.0	979	1.0	996	0.0	1016	0.0
48	936	5.6	979	0.2	1003	0.0	1017	4.3
49	974	0.9	980	0.0	1003	0.0	1026	0.0
50	1021	0.1	1037	1.4	1030	2.2	1027	0.6
51	1069	24.8	1082	1.4	1081	1.5	1074	3.7
52	1079	4.8	1092	1.2	1090	0.2	1084	0.0

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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	1118	0.8	1137	5.2	1138	21.1	1131	19.1
54	1135	46.9	1152	3.7	1151	11.7	1135	112.4
55	1150	3.0	1164	0.4	1165	3.4	1159	31.7
56	1151	2.0	1171	1.2	1165	10.2	1165	10.6
57	1188	0.0	1195	0.1	1210	26.6	1205	25.2
58	1198	0.6	1203	1.6	1213	13.6	1219	31.3
59	1205	21.8	1206	2.0	1222	34.3	1225	16.2
60	1207	49.3	1217	0.9	1223	27.2	1230	81.1
61	1221	0.0	1226	0.2	1230	0.8	1236	1.6
62	1230	28.5	1249	0.2	1246	1.1	1245	12.0
63	1234	2.7	1261	0.9	1251	0.0	1249	2.4
64	1292	94.0	1292	4.2	1309	89.6	1327	126.6
65	1302	161.8	1309	4.7	1331	124.2	1327	303.6
66	1314	70.6	1335	13.6	1334	23.5	1340	18.2
67	1322	39.6	1338	4.0	1339	8.0	1351	51.3
68	1340	21.8	1369	0.2	1370	18.6	1372	8.2
69	1360	1.1	1376	6.6	1381	6.5	1389	55.1
70	1362	67.4	1397	2.0	1388	130.3	1389	389.4
71	1382	1.9	1399	0.5	1413	12.5	1415	7.6
72	1417	1.4	1426	0.4	1430	0.1	1422	0.6
73	1421	5.4	1437	0.0	1434	0.0	1426	3.4
74	1424	0.0	1441	12.1	1446	0.4	1453	10.3
75	1452	11.0	1473	0.2	1468	2.4	1462	107.1
76	1453	0.7	1488	0.1	1470	2.1	1479	6.3
77	1487	4.3	1501	1.9	1491	0.8	1488	195.5
78	1497	91.0	1513	0.1	1506	40.0	1489	0.0
79	1504	9.7	1560	3.0	1513	33.6	1494	20.7
80	1526	140.2	1576	3.6	1542	18.3	1536	69.5
81	1534	53.8	1586	1.9	1543	4.0	1540	15.1
82	1560	151.0	1586	8.3	1552	397.6	1555	589.8
83	1575	15.6	1608	8.0	1580	0.2	1573	6.2
84	1585	4.3	1614	2.1	1594	0.1	1607	4.6
85	3002	7.0	3043	2.1	3071	0.1	3080	0.1
86	3005	14.9	3044	4.7	3072	0.1	3080	0.2
87	3005	111.5	3045	2.4	3073	0.0	3083	5.9
88	3007	4.5	3049	0.4	3076	1.1	3083	0.1
89	3007	3.5	3050	2.8	3077	0.0	3086	0.8
90	3028	19.7	3063	1.5	3087	0.1	3096	1.0
91	3030	6.2	3064	0.2	3088	9.3	3096	6.6
92	3032	177.9	3066	126.7	3090	13.2	3100	1.9
93	3035	322.7	3066	79.7	3092	7.9	3100	2.4
94	3037	4.8	3069	0.9	3095	1.7	3106	3.7
95	3068	4.7	3082	9.6	3107	3.1	3113	1.1
96	3086	68.3	3096	38.6	3120	8.4	3127	0.9