

Harmonic vibrational frequencies of pentacene ($C_{22}H_{14}$) 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	39	0.2	37	0.3	37	0.6	35	1.1
2	70	0.0	71	0.0	71	0.0	70	0.0
3	103	0.0	100	0.0	98	0.0	94	0.0
4	117	1.4	117	1.0	116	0.7	119	0.0
5	149	0.0	149	0.0	149	0.0	147	0.0
6	192	0.3	189	0.9	184	1.7	176	2.3
7	233	0.0	235	0.0	235	0.0	238	0.0
8	239	0.0	239	0.0	241	0.0	239	0.0
9	257	0.0	258	0.0	257	0.0	256	0.0
10	306	0.0	288	0.0	280	0.0	267	0.0
11	326	0.0	345	0.0	352	0.0	353	0.0
12	350	0.0	357	0.1	359	0.1	360	0.4
13	355	0.4	370	0.0	378	0.1	384	0.1
14	449	0.0	448	0.0	438	30.9	422	56.4
15	453	5.0	460	21.8	444	0.0	433	0.0
16	458	0.0	463	0.0	449	0.0	435	0.0
17	463	0.0	467	5.4	462	0.0	455	0.0
18	463	9.0	468	0.0	472	9.1	473	5.1
19	479	48.2	483	7.3	481	0.0	479	3.7
20	507	0.0	507	0.0	501	0.0	489	0.0
21	545	0.0	519	0.0	508	0.0	490	0.0
22	556	0.0	547	0.0	538	0.0	524	0.0
23	577	0.6	572	2.6	575	1.9	578	1.1
24	610	0.0	611	0.0	609	0.0	604	0.0
25	632	16.5	634	4.9	631	0.4	625	3.6
26	634	0.0	642	0.0	633	0.0	627	0.0
27	692	0.0	698	0.0	686	0.0	672	0.0
28	713	62.5	714	0.0	718	0.0	720	0.0
29	713	0.0	724	4.7	728	0.0	721	0.0
30	718	0.0	734	72.5	731	3.5	730	4.8
31	720	0.0	737	0.0	742	0.0	739	0.0
32	728	19.1	740	0.0	753	0.0	743	0.0
33	732	0.0	741	0.0	753	92.5	752	0.0
34	740	0.0	756	0.0	754	0.0	764	0.0
35	745	0.0	760	0.0	757	0.0	765	106.4
36	771	0.0	770	0.0	778	0.0	780	0.0
37	774	14.6	825	0.1	831	0.1	837	0.1
38	785	0.0	827	19.9	851	0.0	866	0.0
39	806	0.0	832	0.0	860	0.0	870	10.7
40	821	0.2	837	0.0	862	16.9	877	0.0
41	824	0.0	862	0.1	869	0.2	899	12.7
42	825	0.0	867	0.0	889	0.0	906	0.5
43	849	132.4	878	0.0	905	0.0	913	0.0
44	854	0.0	898	0.0	909	1.2	923	0.0
45	860	1.0	911	2.0	920	0.0	935	0.0
46	868	0.0	913	103.0	926	0.0	948	0.0
47	905	0.8	919	0.0	941	75.2	973	39.2
48	907	0.0	926	0.0	945	0.0	981	0.0
49	907	18.0	960	0.0	979	0.0	994	0.0
50	921	0.0	961	10.3	980	14.2	996	25.0
51	940	0.0	989	0.0	1011	0.0	1020	48.9
52	940	0.0	989	0.0	1012	0.0	1021	0.0

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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	1007	14.3	992	3.7	1015	0.0	1033	0.0
54	1008	0.0	994	0.0	1015	0.0	1034	0.0
55	1104	8.0	1117	5.5	1120	2.1	1113	0.9
56	1120	0.0	1132	2.9	1135	0.0	1122	0.0
57	1160	2.4	1135	0.0	1173	86.5	1170	0.0
58	1162	0.0	1172	0.0	1185	0.0	1191	37.4
59	1171	0.0	1174	0.2	1187	108.6	1193	0.0
60	1176	69.8	1189	0.0	1188	0.0	1201	5.6
61	1182	0.0	1195	0.0	1199	1.4	1205	317.2
62	1197	0.0	1198	2.4	1204	0.0	1217	0.0
63	1217	0.0	1218	0.0	1231	0.0	1233	0.0
64	1225	146.4	1228	1.3	1237	177.7	1247	4.7
65	1269	0.0	1278	0.0	1281	0.0	1283	0.0
66	1272	1.6	1283	1.0	1285	5.1	1283	21.5
67	1281	24.2	1290	24.0	1296	38.2	1295	0.0
68	1282	0.0	1298	0.0	1297	0.0	1302	0.0
69	1285	0.0	1306	0.0	1298	0.0	1303	27.1
70	1328	0.7	1331	11.6	1345	2.6	1344	1.7
71	1342	1279.5	1351	1.0	1359	945.3	1349	1323.3
72	1359	0.0	1368	0.0	1372	0.0	1366	0.0
73	1364	196.0	1377	0.8	1378	152.0	1390	18.0
74	1368	0.0	1394	1.0	1384	0.0	1402	0.0
75	1374	212.6	1395	0.0	1390	205.2	1416	0.0
76	1396	0.0	1399	0.0	1410	0.0	1435	0.0
77	1436	0.6	1444	0.9	1449	5.6	1437	284.4
78	1442	0.3	1449	1.1	1452	9.1	1451	21.0
79	1466	0.0	1462	0.0	1473	0.0	1455	24.3
80	1487	131.8	1503	2.4	1488	501.3	1481	0.0
81	1488	0.0	1506	0.0	1501	0.0	1503	669.7
82	1489	0.0	1530	1.6	1513	0.0	1504	0.0
83	1512	0.0	1530	0.0	1517	242.2	1509	0.0
84	1514	338.4	1548	0.0	1524	0.0	1527	0.0
85	1518	0.0	1585	0.0	1524	0.0	1529	774.7
86	1554	4.8	1593	0.6	1569	0.6	1552	99.1
87	1571	2.2	1622	0.0	1586	27.5	1570	63.8
88	1586	0.0	1622	11.6	1596	0.0	1576	0.0
89	3008	3.1	3039	2.7	3060	0.2	3065	0.0
90	3009	0.0	3040	0.0	3062	0.0	3067	0.0
91	3010	0.0	3041	0.0	3062	0.0	3068	0.0
92	3011	1.2	3042	5.3	3064	4.3	3069	1.7
93	3012	0.0	3043	12.7	3064	2.1	3069	1.0
94	3013	1.7	3044	0.0	3066	0.0	3070	0.0
95	3016	0.0	3045	50.0	3070	2.5	3082	0.0
96	3016	160.8	3046	0.0	3070	0.0	3082	0.3
97	3018	1.5	3049	5.2	3073	4.9	3084	1.2
98	3021	0.0	3049	0.0	3073	0.0	3084	0.0
99	3032	0.0	3064	0.1	3088	0.0	3098	0.0
100	3033	216.1	3064	81.3	3088	14.7	3098	1.2
101	3051	402.8	3079	142.6	3100	50.4	3109	0.0
102	3051	0.0	3079	0.0	3100	0.0	3109	0.5