

Harmonic vibrational frequencies of anthracene (C₁₄H₁₀) 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	92	0.5	90	1.0	86	1.9	80	3.0
2	116	0.0	121	0.0	118	0.0	115	0.0
3	231	2.4	232	0.0	218	0.0	201	0.0
4	249	0.0	232	1.3	231	0.4	233	0.1
5	253	0.0	267	0.0	267	0.0	258	0.0
6	335	0.0	379	0.0	377	0.3	367	3.1
7	387	0.0	390	0.0	383	0.0	376	0.0
8	387	0.0	391	0.0	387	0.0	384	0.0
9	459	5.1	470	17.4	438	31.2	419	50.7
10	464	0.0	475	0.0	454	0.0	422	0.0
11	533	0.0	499	0.0	478	0.0	439	0.0
12	533	0.0	530	0.0	517	0.0	486	0.0
13	571	0.0	584	0.0	555	0.0	511	0.0
14	609	2.3	613	7.5	606	2.0	596	12.5
15	624	0.0	638	0.0	625	0.0	615	0.0
16	652	0.5	651	0.6	658	0.0	665	0.9
17	683	50.7	729	75.8	724	0.0	692	0.0
18	710	0.0	743	0.0	743	0.0	733	0.0
19	717	0.0	744	0.0	747	0.0	739	0.0
20	728	0.0	759	0.0	753	95.5	761	0.0
21	732	0.0	767	0.0	762	0.0	768	106.4
22	752	0.0	796	0.0	806	5.1	804	19.3
23	770	94.6	834	0.0	856	0.0	875	0.0
24	789	68.4	855	0.0	888	0.0	901	0.2
25	803	0.0	884	64.7	905	0.6	911	0.0
26	831	0.0	908	1.7	912	38.3	915	0.0
27	845	0.0	909	0.0	917	0.0	953	16.8
28	849	26.9	918	0.0	938	0.0	982	0.0
29	894	0.0	955	0.0	978	0.0	998	0.0
30	900	0.0	961	8.3	985	8.8	1010	8.4
31	901	0.0	989	0.0	1019	0.0	1018	0.0
32	901	0.0	990	0.0	1021	0.0	1018	64.7
33	1017	32.4	1000	3.2	1023	6.9	1040	0.0
34	1019	0.0	1005	0.0	1024	0.0	1042	0.0
35	1074	0.0	1100	0.0	1095	0.0	1055	0.0
36	1120	11.6	1156	4.7	1139	0.3	1106	28.3
37	1150	3.2	1158	3.4	1182	11.3	1177	0.0
38	1162	0.0	1169	1.0	1194	0.0	1192	60.8
39	1170	0.0	1181	0.0	1196	140.0	1204	0.0
40	1189	42.9	1202	0.0	1199	0.0	1222	251.4
41	1239	0.0	1266	0.0	1255	0.0	1255	0.0
42	1257	9.1	1274	10.1	1279	22.6	1268	24.3
43	1263	0.0	1282	0.0	1285	0.0	1286	0.0
44	1275	1.8	1311	2.0	1298	1.6	1306	8.5
45	1323	371.0	1343	4.1	1339	355.6	1334	302.6
46	1347	0.0	1383	0.1	1368	0.0	1380	0.0
47	1375	149.6	1385	0.0	1393	131.4	1405	0.0
48	1385	0.0	1397	0.0	1408	0.0	1419	0.0
49	1434	1.0	1455	3.6	1455	21.9	1439	107.6
50	1444	3.7	1456	2.0	1458	59.3	1444	84.7
51	1458	0.0	1482	0.0	1497	0.0	1469	310.6
52	1479	0.0	1534	4.9	1506	0.0	1480	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	1509	212.3	1541	0.0	1523	75.5	1504	0.0
54	1514	0.0	1578	0.0	1527	0.0	1542	121.7
55	1526	0.0	1617	0.0	1542	0.0	1549	194.9
56	1547	5.9	1620	7.8	1564	62.0	1553	0.0
57	2992	0.6	3039	10.8	3065	0.3	3065	6.8
58	2993	0.0	3041	0.0	3067	0.0	3066	0.0
59	2997	0.0	3044	0.0	3076	0.0	3082	0.0
60	2999	51.2	3044	18.9	3076	0.7	3082	13.8
61	3002	44.7	3048	0.0	3078	2.1	3083	0.0
62	3006	0.0	3049	0.0	3079	0.0	3083	0.0
63	3016	0.0	3063	0.0	3093	0.0	3100	0.0
64	3017	300.9	3064	81.1	3093	2.6	3100	17.8
65	3035	293.6	3078	95.4	3106	8.4	3110	35.9
66	3037	0.0	3079	0.0	3106	0.0	3110	0.0