

Harmonic vibrational frequencies of naphthalene (C<sub>10</sub>H<sub>8</sub>) 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 <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )
1	167	0.0	171	1.9	156	3.2	138	3.2
2	179	2.3	185	0.0	180	0.0	171	0.0
3	308	0.0	361	1.3	355	0.1	346	0.0
4	360	4.7	388	0.0	368	0.0	351	1.2
5	461	3.3	473	0.0	421	24.1	353	35.9
6	502	0.0	479	16.1	437	0.0	370	0.0
7	506	0.0	512	0.0	473	0.0	407	0.0
8	507	0.0	513	0.0	507	0.0	433	0.0
9	583	0.0	629	0.0	558	0.0	497	0.0
10	607	9.2	632	3.2	609	7.3	596	6.1
11	649	0.0	718	0.0	729	0.0	692	0.0
12	699	0.0	751	0.0	739	0.0	743	123.5
13	699	120.1	772	0.0	752	0.0	747	0.0
14	710	0.0	788	111.3	766	115.2	756	0.0
15	727	0.0	797	0.2	799	0.0	793	0.0
16	749	0.0	838	0.0	859	0.0	886	0.0
17	765	21.2	885	0.0	922	0.0	898	0.0
18	784	4.7	940	0.0	931	0.0	968	0.0
19	797	0.0	943	0.0	963	0.0	969	42.8
20	862	0.0	963	4.2	987	2.2	985	0.0
21	871	0.0	986	0.0	1008	21.5	991	0.0
22	891	0.0	993	0.0	1018	0.0	1019	0.1
23	996	86.7	1010	4.1	1022	0.0	1027	0.0
24	1026	0.0	1019	0.0	1038	0.0	1039	0.0
25	1050	0.0	1131	3.2	1097	0.0	1040	0.0
26	1088	15.6	1155	0.0	1103	7.1	1055	79.5
27	1149	0.0	1169	1.2	1182	49.8	1195	53.5
28	1152	11.6	1173	0.0	1191	0.0	1203	0.0
29	1199	115.3	1209	1.2	1218	193.6	1221	0.0
30	1207	0.0	1256	0.0	1243	0.0	1234	205.5
31	1247	10.0	1270	8.2	1283	9.0	1288	5.8
32	1329	0.0	1358	1.5	1364	0.0	1358	0.0
33	1363	38.6	1363	0.0	1375	20.3	1359	0.0
34	1376	0.0	1399	3.2	1410	16.2	1409	93.3
35	1379	1.4	1462	0.0	1440	0.0	1426	0.0
36	1421	0.0	1463	0.0	1460	0.0	1436	148.4
37	1442	0.0	1508	9.1	1470	0.0	1449	261.4
38	1490	12.8	1561	0.0	1501	97.8	1467	0.0
39	1495	107.9	1593	6.3	1524	17.6	1554	29.6
40	1550	0.0	1618	0.0	1566	0.0	1579	0.0
41	2974	0.0	3042	0.0	3079	0.0	3071	0.0
42	2976	0.5	3043	9.6	3081	0.0	3072	0.1
43	2986	93.4	3045	1.2	3081	1.4	3074	49.3
44	2992	0.0	3049	0.0	3083	0.0	3074	0.0
45	3001	0.0	3061	0.0	3099	0.0	3097	0.0
46	3006	325.5	3062	77.8	3099	0.0	3097	37.4
47	3019	247.6	3077	71.4	3111	0.1	3107	79.6
48	3026	0.0	3078	0.0	3111	0.0	3107	0.0