

Harmonic vibrational frequencies of acenaphthylene (C₁₂H₈) 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	179	2.4	159	5.2	168	8.8	94	8.0
2	210	0.0	210	0.0	195	0.0	120	0.0
3	220	0.6	226	3.4	200	9.5	213	0.7
4	344	0.0	368	0.0	353	0.0	258	0.0
5	411	7.9	415	1.5	413	0.0	321	9.8
6	465	4.6	456	0.0	438	50.3	373	0.0
7	488	0.3	460	1.2	449	1.2	391	0.0
8	506	0.4	512	1.6	484	0.0	414	0.0
9	541	1.6	553	3.0	505	0.0	432	0.0
10	552	0.0	574	0.0	534	0.9	497	138.3
11	602	0.4	601	0.1	542	3.4	504	0.0
12	642	0.0	646	0.6	613	0.0	570	0.0
13	647	0.2	662	0.0	655	0.0	576	0.0
14	667	31.5	688	0.0	694	1.9	707	0.0
15	686	0.2	730	42.3	745	47.1	717	1.4
16	687	0.0	757	0.0	773	0.0	744	151.2
17	713	79.8	773	27.0	777	2.9	748	0.0
18	763	0.0	804	0.4	786	0.4	756	0.0
19	785	1.7	835	65.8	849	22.4	868	0.0
20	786	0.0	866	3.3	851	91.6	883	0.0
21	794	0.6	904	0.0	915	0.0	902	372.5
22	801	22.7	919	2.4	949	0.0	947	0.0
23	856	0.1	926	0.0	959	0.2	965	0.0
24	889	0.0	971	0.0	1010	0.0	973	1.3
25	896	0.5	979	1.9	1012	72.8	977	0.0
26	1006	4.7	998	2.7	1016	5.9	979	7.9
27	1018	13.1	1011	0.0	1016	0.2	986	0.0
28	1035	0.6	1031	2.7	1045	0.8	1016	0.0
29	1060	29.4	1092	2.1	1065	28.2	1019	0.0
30	1090	0.7	1093	12.3	1093	185.6	1025	63.1
31	1155	0.2	1167	5.3	1118	0.5	1093	0.0
32	1175	15.2	1189	4.0	1191	35.4	1130	115.9
33	1179	6.9	1201	2.1	1213	0.7	1134	0.2
34	1211	15.8	1225	4.1	1232	29.9	1207	0.0
35	1253	0.3	1247	0.4	1251	54.4	1277	219.0
36	1305	13.6	1305	1.1	1298	35.6	1282	15.5
37	1305	25.3	1352	2.0	1303	3.7	1294	0.0
38	1356	4.1	1385	5.0	1333	6.4	1348	10.7
39	1382	0.6	1417	15.5	1354	9.6	1356	0.0
40	1403	3.8	1424	23.1	1400	39.3	1382	0.0
41	1411	13.5	1447	22.4	1410	0.5	1422	149.6
42	1435	7.2	1476	6.7	1446	12.4	1430	11.6
43	1466	8.2	1492	10.1	1483	7.4	1446	0.0
44	1511	13.1	1588	0.0	1538	11.4	1470	0.0
45	1520	7.8	1600	0.1	1562	104.7	1541	0.6
46	1566	13.1	1607	2.5	1586	14.5	1638	0.0
47	2980	25.3	3047	0.3	3081	0.0	3093	0.0
48	2981	13.1	3047	0.1	3082	0.0	3094	1.3
49	3005	65.8	3057	4.9	3091	0.0	3100	16.4
50	3007	83.8	3058	36.9	3091	0.0	3100	0.0
51	3020	208.1	3073	69.2	3104	1.1	3105	0.0
52	3025	90.5	3074	15.4	3104	0.4	3106	75.9

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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	3038	45.7	3098	1.9	3124	3.9	3109	47.1
54	3064	101.7	3121	26.1	3138	1.4	3110	0.0