

Harmonic vibrational frequencies of acenaphthene (C₁₂H₁₀) 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	49	0.0	98	0.0	125	0.0	143	0.0
2	165	2.2	162	1.3	157	2.7	152	4.2
3	190	2.5	214	7.0	198	10.0	176	14.7
4	207	0.0	236	0.0	228	0.0	221	0.0
5	321	0.0	415	1.2	408	0.5	389	0.0
6	409	3.2	438	0.0	419	0.0	402	0.1
7	426	9.1	443	0.6	435	5.5	406	5.6
8	498	0.5	468	0.1	445	0.7	428	3.3
9	499	0.0	505	0.0	477	0.0	457	5.0
10	520	1.0	544	0.9	514	0.0	472	3.2
11	532	4.5	554	0.2	540	0.0	532	0.8
12	574	0.0	622	0.0	586	0.0	533	0.0
13	614	1.3	623	0.0	621	0.8	618	4.3
14	634	4.2	659	2.9	649	4.3	643	7.9
15	661	0.0	751	0.0	714	13.1	666	19.1
16	691	89.1	755	11.2	764	47.0	733	34.0
17	724	0.2	789	60.2	766	0.0	779	0.0
18	726	0.0	803	0.5	803	0.2	798	0.0
19	771	8.6	825	0.9	825	0.0	825	0.0
20	790	6.2	844	23.1	841	48.2	841	74.3
21	794	0.6	881	0.0	904	0.0	909	0.0
22	812	2.3	905	0.1	916	4.9	924	21.2
23	843	0.0	907	0.7	942	0.1	961	0.0
24	854	1.0	968	0.0	984	0.0	980	10.2
25	886	1.6	977	1.9	993	0.3	990	0.1
26	967	0.2	983	0.3	1009	0.0	997	7.5
27	992	55.3	1015	2.2	1012	0.3	1034	0.0
28	1006	0.0	1017	0.0	1014	18.2	1038	0.1
29	1020	19.0	1040	0.1	1052	4.7	1041	45.3
30	1036	9.5	1086	0.8	1091	5.3	1073	38.2
31	1119	0.3	1153	0.6	1149	1.1	1096	0.0
32	1141	6.6	1169	0.1	1168	0.0	1127	2.4
33	1161	4.5	1181	1.2	1177	0.0	1128	163.6
34	1169	25.7	1215	0.0	1182	120.2	1186	24.1
35	1203	0.0	1216	1.4	1193	4.8	1195	2.3
36	1209	58.5	1225	0.0	1221	2.1	1208	30.6
37	1209	2.3	1226	0.2	1230	83.5	1234	124.0
38	1235	0.0	1249	2.2	1266	24.8	1276	76.9
39	1251	78.4	1285	2.0	1300	6.1	1297	33.2
40	1336	0.1	1353	1.2	1363	10.8	1346	12.5
41	1339	16.4	1362	13.1	1370	1.2	1358	269.7
42	1352	31.0	1420	2.6	1406	42.3	1376	11.4
43	1394	2.4	1433	0.5	1415	38.5	1387	43.3
44	1421	10.4	1453	1.0	1443	60.3	1405	36.0
45	1422	0.0	1472	0.4	1447	1.2	1423	33.1
46	1461	63.3	1479	2.0	1448	0.6	1426	213.5
47	1482	52.0	1490	4.6	1459	8.3	1438	158.6
48	1487	5.2	1583	6.4	1502	110.4	1475	4.7
49	1490	29.0	1591	16.1	1504	15.3	1532	46.2
50	1560	5.2	1607	8.2	1591	3.8	1602	1.4
51	2814	140.6	2913	19.7	2920	0.8	2865	57.2
52	2818	0.0	2925	48.3	2924	19.7	2866	337.3

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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	2844	306.5	2940	0.0	2948	0.0	2882	0.0
54	2855	173.9	2960	39.9	2959	0.0	2883	52.5
55	2976	7.1	3043	0.8	3082	0.3	3078	0.1
56	2978	15.3	3043	1.0	3082	0.0	3078	20.0
57	2996	97.9	3054	5.6	3090	0.0	3093	1.5
58	2999	104.1	3055	44.6	3090	0.3	3093	21.0
59	3015	225.0	3069	72.3	3102	1.6	3105	47.0
60	3020	84.3	3071	16.4	3103	0.0	3105	3.2