

Harmonic vibrational frequencies of hexacene ( $C_{26}H_{16}$ ) 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	29	0.1	26	0.2	27	0.3	26	0.7
2	58	0.0	59	0.0	59	0.0	58	0.0
3	75	0.0	72	0.0	72	0.0	69	0.0
4	89	1.4	89	0.8	88	0.8	91	0.0
5	122	0.0	122	0.0	122	0.0	121	0.0
6	142	0.3	139	0.7	136	1.3	131	1.8
7	186	0.0	187	0.0	188	0.0	190	0.0
8	194	0.0	193	0.0	194	0.0	193	0.0
9	219	0.0	220	0.0	215	0.0	208	0.0
10	222	0.0	220	0.0	219	0.0	219	0.0
11	273	0.0	275	0.0	277	0.0	278	0.0
12	291	0.4	292	0.2	294	0.1	286	1.1
13	320	0.1	302	0.2	297	0.7	296	0.5
14	345	0.0	366	0.0	373	0.0	377	0.0
15	353	0.0	368	0.0	377	0.0	385	0.0
16	386	0.0	387	0.0	387	0.0	386	0.0
17	417	55.2	420	6.3	419	0.4	418	0.8
18	451	5.8	457	21.2	438	31.5	425	56.1
19	457	0.0	460	0.0	445	0.0	433	1.2
20	458	1.3	462	1.6	457	0.0	449	0.0
21	463	11.1	463	8.7	469	12.8	466	0.0
22	463	0.0	467	0.0	471	0.2	468	8.0
23	472	0.0	472	0.1	472	0.0	471	0.3
24	490	0.0	489	0.0	482	0.0	474	0.0
25	545	0.0	523	0.0	514	0.0	499	0.0
26	551	0.0	540	0.0	532	0.0	522	0.0
27	561	1.5	556	3.3	557	4.4	559	0.7
28	570	0.0	572	0.0	570	0.0	568	0.0
29	625	35.6	626	8.7	625	0.7	620	4.3
30	635	0.7	637	0.0	634	0.0	629	0.0
31	635	0.0	642	0.0	635	0.0	630	0.0
32	663	0.0	662	0.0	665	0.0	663	0.0
33	683	0.0	684	0.0	674	0.0	667	0.0
34	709	0.0	723	0.0	716	0.0	709	0.0
35	719	0.0	724	6.7	730	4.2	729	5.2
36	723	72.2	734	0.0	736	0.0	735	0.0
37	728	11.2	735	0.0	739	0.0	736	0.0
38	728	0.0	738	77.5	745	0.0	745	0.0
39	728	0.0	741	0.0	751	0.0	750	0.0
40	741	0.0	744	0.0	752	92.1	755	0.0
41	745	0.0	756	0.0	757	0.0	762	104.1
42	747	0.0	758	0.0	759	0.0	762	0.0
43	771	0.0	790	0.0	794	0.0	797	0.3
44	789	0.0	806	0.0	812	0.0	814	10.3
45	792	0.0	812	0.0	839	0.0	845	0.0
46	806	0.0	831	0.0	847	0.0	863	0.0
47	810	0.0	834	0.0	849	0.0	869	0.0
48	815	6.5	835	0.0	855	0.0	879	0.0
49	823	0.0	856	20.8	876	0.0	882	0.0
50	830	0.0	856	0.0	878	0.0	896	0.0
51	845	0.0	872	0.0	883	25.1	911	23.7
52	849	0.0	883	0.0	903	0.0	916	0.4

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Table 1 - continued from previous page

Numb. of the mode	Anion		Neutral		Cation		Dication	
	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )
53	865	161.6	892	0.0	918	0.0	919	0.0
54	870	0.0	905	0.0	918	1.8	925	0.0
55	870	0.0	917	126.1	922	0.0	944	0.0
56	878	0.0	918	2.6	927	0.0	952	0.0
57	914	2.5	920	0.0	943	95.6	973	56.8
58	919	0.0	923	0.0	945	0.0	978	0.0
59	919	0.0	961	0.0	977	0.0	991	0.0
60	920	15.8	961	10.2	978	14.3	992	25.8
61	950	0.0	989	0.0	1007	1.7	1017	25.3
62	950	0.0	989	0.0	1007	0.0	1017	0.0
63	1003	7.8	990	3.8	1012	0.0	1029	0.0
64	1004	0.0	991	0.0	1012	0.0	1029	0.0
65	1112	0.0	1120	2.3	1126	0.0	1120	0.0
66	1116	13.6	1122	0.0	1130	3.1	1125	0.0
67	1159	0.5	1128	6.5	1166	135.4	1166	0.0
68	1164	0.0	1172	0.2	1184	75.5	1188	15.3
69	1169	79.3	1172	0.0	1184	0.0	1192	0.0
70	1172	0.0	1186	0.0	1184	0.0	1195	3.0
71	1177	3.2	1186	0.0	1193	4.4	1198	302.5
72	1189	0.0	1192	1.4	1194	0.0	1204	0.0
73	1190	0.0	1201	0.0	1202	0.0	1208	0.0
74	1207	387.9	1211	2.2	1215	434.9	1228	192.1
75	1237	0.1	1234	0.6	1249	0.2	1252	2.9
76	1244	0.0	1245	0.0	1256	0.0	1261	0.0
77	1272	2.1	1280	0.0	1283	2.6	1284	0.0
78	1273	0.0	1281	0.0	1283	0.0	1286	17.7
79	1278	0.0	1289	0.0	1292	0.0	1295	0.0
80	1283	40.8	1293	35.7	1298	50.9	1306	21.3
81	1292	6.9	1306	2.8	1306	119.4	1308	0.5
82	1295	161.2	1314	0.4	1306	10.0	1310	9.0
83	1343	0.0	1326	13.4	1357	0.0	1357	0.0
84	1353	1865.3	1362	0.0	1366	869.3	1357	1829.8
85	1361	365.3	1363	0.0	1374	748.0	1365	0.0
86	1361	0.0	1376	0.6	1375	0.0	1390	0.0
87	1365	0.0	1381	0.0	1376	0.0	1394	42.9
88	1372	73.5	1396	0.0	1386	213.8	1401	0.0
89	1377	0.0	1396	2.0	1391	0.0	1416	8.6
90	1399	0.3	1401	1.0	1410	4.1	1430	493.1
91	1435	0.0	1441	0.0	1446	0.0	1431	0.0
92	1442	0.0	1447	0.0	1450	0.0	1450	0.0
93	1462	0.1	1458	1.4	1467	22.7	1453	0.0
94	1479	0.0	1491	0.0	1485	0.0	1474	168.4
95	1483	0.0	1495	0.0	1492	911.4	1494	0.0
96	1486	0.0	1512	1.2	1496	0.0	1504	8.4
97	1494	364.3	1527	2.1	1501	0.0	1504	0.0
98	1507	0.1	1531	0.0	1517	2.2	1507	988.5
99	1517	199.0	1536	0.5	1520	131.5	1521	0.0
100	1519	0.0	1569	0.0	1522	0.0	1522	776.8
101	1545	39.9	1581	0.0	1567	0.9	1554	0.0
102	1559	0.0	1602	0.7	1567	0.0	1562	143.5
103	1590	2.1	1620	13.0	1599	18.4	1581	3.3
104	1592	0.0	1624	0.0	1603	0.0	1586	0.0
105	3012	0.0	3039	0.0	3058	0.0	3064	0.0
106	3014	4.7	3040	5.4	3059	0.7	3066	0.2

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Table 1 - continued from previous page

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	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )
107	3014	1.3	3041	1.5	3060	0.2	3066	0.1
108	3015	0.0	3042	0.0	3061	0.0	3067	0.0
109	3016	0.0	3042	0.0	3061	0.0	3068	0.0
110	3016	2.8	3044	3.9	3062	6.6	3068	0.1
111	3018	0.0	3044	7.9	3063	3.7	3069	1.0
112	3019	1.5	3045	0.0	3065	0.0	3070	0.0
113	3021	186.7	3045	71.1	3068	3.1	3080	0.0
114	3022	0.0	3047	0.0	3068	0.0	3080	0.0
115	3023	1.4	3049	11.1	3071	8.2	3082	2.9
116	3026	0.0	3049	0.0	3071	0.0	3082	0.0
117	3038	0.0	3064	0.0	3085	0.0	3096	0.0
118	3038	190.5	3064	81.2	3085	20.8	3096	0.0
119	3055	461.3	3079	162.3	3098	80.9	3107	2.9
120	3056	0.0	3079	0.0	3098	0.0	3107	0.0