

Harmonic vibrational frequencies of quaterrylene ( $C_{40}H_{20}$ ) 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	21	0.0	13	0.0	21	0.4	19	1.0
2	22	0.0	21	0.1	24	0.0	21	0.0
3	33	0.0	25	0.0	41	0.0	43	0.0
4	38	0.0	29	0.0	53	0.0	50	0.0
5	54	0.0	51	0.0	56	0.0	63	0.0
6	95	0.2	92	0.1	95	0.3	91	0.7
7	113	0.1	108	0.0	114	0.6	113	0.9
8	114	0.0	112	0.3	121	0.0	124	0.0
9	161	0.0	153	0.0	158	0.0	158	0.1
10	173	0.0	166	0.0	169	0.0	167	0.0
11	178	5.1	173	8.1	172	12.1	167	16.8
12	182	0.0	181	0.0	183	0.0	184	0.0
13	198	0.0	196	0.0	198	0.0	197	0.0
14	205	0.0	210	0.0	209	0.0	207	0.0
15	206	0.0	213	0.0	214	0.0	215	0.0
16	254	0.0	254	0.0	252	0.0	249	0.0
17	261	0.0	261	0.0	258	0.0	256	0.0
18	296	1.3	294	0.1	296	0.0	293	0.0
19	308	1.4	312	1.7	303	1.9	295	1.9
20	310	0.0	318	0.0	316	0.0	313	0.0
21	351	3.1	352	3.1	354	18.2	351	0.0
22	361	0.0	360	0.0	358	0.0	355	19.6
23	361	0.0	365	0.0	363	0.0	365	0.0
24	408	0.0	405	0.0	410	0.0	409	0.0
25	409	1.2	408	0.0	411	0.3	410	0.0
26	411	0.0	423	0.0	418	0.0	412	1.3
27	437	0.0	436	0.0	436	0.0	434	0.0
28	442	1.9	441	4.7	441	12.2	439	26.1
29	462	0.0	460	0.1	457	0.0	445	0.0
30	479	0.5	466	0.0	458	1.5	450	5.3
31	479	0.0	469	0.0	460	0.0	450	0.0
32	485	0.1	473	0.1	473	0.3	476	1.0
33	488	0.0	474	0.0	486	0.0	486	0.0
34	499	0.0	490	0.0	489	0.0	496	0.0
35	504	0.0	506	0.0	509	0.0	509	0.0
36	513	63.1	518	4.5	517	0.4	510	0.0
37	515	0.0	528	0.0	520	0.0	516	27.0
38	537	0.0	538	0.0	535	0.0	530	0.0
39	541	0.2	540	0.9	538	2.4	534	4.6
40	542	0.0	545	0.0	545	0.0	544	0.0
41	543	0.0	561	0.0	559	3.0	549	2.3
42	562	9.9	562	0.0	560	0.0	555	0.0
43	563	0.0	568	3.4	563	0.0	562	0.0
44	568	0.5	568	5.2	567	4.3	563	0.1
45	579	0.1	580	0.2	575	0.0	570	0.0
46	599	0.0	597	0.0	590	0.0	582	0.0
47	622	0.0	628	0.0	623	0.0	616	0.0
48	625	0.0	629	0.0	624	0.0	620	0.0
49	635	0.0	637	0.0	635	0.0	632	0.0
50	643	0.0	648	0.0	656	0.0	650	18.5
51	654	9.8	662	0.0	657	12.6	664	0.0
52	664	0.0	664	8.0	665	0.0	665	0.0

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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	677	0.9	678	0.0	678	5.8	673	36.2
54	677	0.0	681	0.0	690	0.0	688	0.0
55	679	0.0	696	0.0	692	0.0	702	0.0
56	707	0.1	709	0.5	708	0.1	705	0.1
57	740	62.0	754	0.0	747	0.0	740	0.0
58	741	0.0	754	50.7	748	52.6	741	50.1
59	742	0.0	761	0.0	770	0.1	770	0.0
60	743	0.0	762	0.0	772	0.0	776	0.0
61	769	12.6	774	1.4	775	0.0	784	0.0
62	773	0.0	782	0.0	781	0.0	788	0.0
63	778	0.0	786	0.0	785	0.0	788	0.0
64	786	3.6	788	64.6	788	17.7	788	8.5
65	791	207.3	794	0.0	795	0.0	795	0.0
66	792	0.0	798	10.0	799	4.5	799	1.8
67	793	0.0	806	0.0	806	0.0	805	0.0
68	793	0.0	815	7.1	815	1.4	812	0.0
69	795	84.7	818	246.3	815	248.3	815	250.7
70	803	0.0	822	0.0	826	0.0	830	0.0
71	809	6.1	825	0.0	830	0.0	833	0.0
72	812	0.0	829	0.0	831	0.0	837	0.0
73	826	0.0	837	0.0	840	0.0	844	2.9
74	828	11.8	839	0.0	841	0.9	845	0.0
75	831	0.0	860	2.5	855	2.3	847	18.1
76	831	0.0	882	0.0	893	0.0	896	0.0
77	855	0.0	882	0.0	905	0.0	932	0.0
78	855	2.5	887	0.0	905	0.0	932	0.0
79	855	0.0	902	0.4	926	3.0	953	0.0
80	887	0.0	902	0.0	926	0.0	953	5.3
81	905	0.0	934	0.0	958	0.0	958	0.0
82	912	0.0	941	0.0	961	0.0	976	0.0
83	923	0.0	947	0.0	962	0.0	978	0.0
84	927	0.1	951	0.0	970	0.0	987	59.0
85	944	0.0	963	0.0	972	0.0	988	0.0
86	944	0.0	971	0.0	982	10.2	989	0.0
87	950	0.0	971	0.0	990	0.0	989	21.5
88	950	2.5	976	21.7	990	0.0	1009	0.0
89	958	0.0	979	0.0	999	5.5	1009	0.0
90	974	68.1	979	2.4	999	0.0	1019	0.0
91	996	11.0	1005	1.5	999	0.8	1019	0.0
92	1035	0.0	1044	0.0	1042	0.0	1035	0.0
93	1052	7.4	1053	0.0	1058	0.1	1056	0.6
94	1054	0.0	1055	2.5	1063	0.0	1066	0.0
95	1075	0.0	1072	0.0	1079	0.0	1079	0.0
96	1094	21.3	1096	0.0	1101	0.6	1104	31.9
97	1095	0.0	1096	2.6	1101	0.0	1104	0.0
98	1127	1.5	1140	2.6	1136	4.8	1127	4.9
99	1142	0.0	1149	0.0	1151	0.0	1147	0.0
100	1156	1.3	1159	0.0	1162	2.9	1154	9.6
101	1156	20.5	1167	0.4	1167	1.0	1156	0.1
102	1164	0.0	1170	0.0	1171	0.0	1171	0.1
103	1166	0.0	1177	3.2	1177	0.0	1180	0.0
104	1177	10.0	1181	0.0	1184	18.1	1185	166.6
105	1191	0.1	1199	0.1	1202	0.0	1204	0.0
106	1192	0.0	1200	0.0	1203	0.0	1205	2.0

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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. ( $\text{km mol}^{-1}$ )
107	1204	8.3	1208	0.0	1217	0.0	1223	0.0
108	1208	0.0	1211	8.8	1219	14.3	1225	46.9
109	1215	0.0	1216	3.9	1225	47.3	1230	0.0
110	1215	0.0	1220	0.0	1228	0.0	1232	111.9
111	1222	0.0	1225	0.0	1233	0.0	1236	145.9
112	1226	20.9	1238	5.3	1243	60.5	1238	0.1
113	1256	0.0	1256	0.0	1264	0.0	1278	0.0
114	1258	55.7	1272	1.1	1274	50.9	1279	3011.1
115	1266	1009.6	1277	0.0	1274	1085.2	1282	52.9
116	1282	0.0	1285	13.0	1292	0.0	1294	0.0
117	1282	0.0	1296	0.0	1296	0.0	1302	0.0
118	1297	0.0	1297	0.0	1307	0.0	1305	0.0
119	1299	30.6	1297	0.5	1310	5.0	1326	34.2
120	1306	2.1	1309	0.0	1321	0.4	1334	33.4
121	1312	44.0	1317	0.0	1326	46.1	1344	42.9
122	1315	0.0	1318	5.5	1327	0.0	1345	24.2
123	1335	0.0	1339	0.0	1347	0.2	1348	0.0
124	1335	0.1	1339	3.2	1351	0.0	1355	0.0
125	1336	144.7	1349	0.0	1352	1.5	1362	573.8
126	1338	0.0	1350	26.2	1355	102.8	1369	0.0
127	1341	66.8	1354	1.8	1357	0.0	1375	0.0
128	1358	0.0	1354	0.0	1367	0.0	1385	0.0
129	1380	44.5	1387	123.8	1390	110.9	1390	57.9
130	1386	0.0	1387	0.0	1398	0.0	1407	0.0
131	1412	5.7	1414	0.0	1423	2.1	1421	0.9
132	1420	1.6	1418	0.0	1431	0.0	1425	5.0
133	1423	0.0	1445	15.1	1436	0.0	1442	0.0
134	1439	0.0	1448	0.0	1449	0.0	1447	0.0
135	1442	13.5	1450	0.1	1451	49.7	1451	0.0
136	1444	0.0	1453	0.0	1455	0.0	1454	9.6
137	1445	4.4	1461	2.8	1457	0.0	1459	40.3
138	1449	0.0	1463	0.0	1458	4.6	1461	0.0
139	1486	25.1	1494	19.6	1490	10.5	1494	34.9
140	1493	0.0	1497	0.0	1495	0.0	1494	2.9
141	1511	0.3	1512	0.1	1514	0.6	1509	44.8
142	1525	321.8	1527	0.0	1534	282.9	1512	4.7
143	1534	0.0	1531	0.0	1536	441.7	1531	0.0
144	1537	771.8	1551	16.2	1540	0.0	1539	0.0
145	1538	0.0	1563	0.0	1540	0.0	1548	517.9
146	1538	0.0	1566	56.3	1545	0.0	1550	0.0
147	1547	0.8	1568	0.5	1554	5.3	1552	2126.1
148	1560	0.0	1572	0.0	1563	0.0	1553	6.8
149	1560	0.0	1581	0.0	1563	0.0	1559	0.0
150	1564	5.6	1581	44.9	1564	129.2	1563	0.0
151	1569	0.0	1582	0.0	1565	0.0	1576	0.0
152	1572	95.7	1586	0.7	1582	47.5	1579	37.7
153	1572	0.0	1599	10.4	1582	0.0	1581	0.0
154	1585	15.8	1599	0.0	1583	2.5	1590	446.9
155	3025	0.0	3049	0.1	3069	0.0	3078	0.1
156	3025	61.4	3049	8.6	3069	0.6	3078	0.0
157	3026	62.5	3051	6.6	3071	0.1	3080	0.0
158	3026	0.0	3051	0.0	3071	0.0	3080	0.1
159	3046	0.0	3066	0.0	3086	0.0	3095	0.1
160	3046	62.6	3067	26.1	3086	7.6	3095	0.0

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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. ( $\text{km mol}^{-1}$ )
161	3050	576.7	3068	305.6	3086	109.7	3096	0.0
162	3050	0.0	3069	0.0	3087	0.0	3096	0.0
163	3059	3.5	3072	0.0	3093	7.0	3101	13.1
164	3059	0.0	3073	9.8	3093	0.0	3101	0.0
165	3065	0.1	3079	9.0	3099	7.0	3107	0.9
166	3065	0.0	3079	0.0	3099	0.0	3107	0.0
167	3078	0.0	3087	0.0	3104	0.0	3111	0.0
168	3079	2.2	3087	13.6	3104	14.1	3111	4.0
169	3087	30.8	3095	23.0	3112	10.3	3120	1.0
170	3088	0.0	3095	0.0	3112	0.0	3120	0.0
171	3092	0.0	3101	0.0	3119	0.0	3127	0.0
172	3092	46.3	3101	35.6	3119	29.4	3127	8.3
173	3097	217.4	3106	119.0	3124	55.4	3131	17.6
174	3098	0.0	3106	0.0	3124	0.0	3132	0.0