Harmonic vibrational frequencies of ovalene ($C_{32}H_{14}$) 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	60	0.0	61	0.0	62	0.0	60	1.7
2	63	0.2	62	0.5	62	1.0	62	0.0
3	107	0.9	105	3.4	102	7.4	99	13.0
4	124	0.0	125	0.0	124	0.0	121	0.0
5	151	0.0	152	0.0	152	0.0	150	0.0
6	196	0.0	193	0.0	190	0.0	186	0.0
7	205	0.0	210	0.0	210	0.5	208	1.7
8	255	0.0	255	0.0	251	0.0	246	0.0
9	265	0.0	268	0.0	263	0.0	256	0.0
10	272	15.1	275	3.7	273	1.1	273	0.0
11	309	0.0	312	0.0	307	0.0	300	0.0
12	316	0.0	318	0.0	317	0.0	307	0.0
13	327	4.8	323	0.0	318	0.0	318	0.0
14	328	0.0	332	0.0	328	0.0	321	0.0
15	328	0.0	339	5.2	338	0.0	335	0.0
16	337	0.0	340	0.0	341	5.1	340	4.5
17	391	10.8	391	3.9	391	8.3	390	9.7
18	410	0.0	410	0.0	411	0.0	411	0.0
19	410	0.1	424	2.2	421	0.0	416	0.3
20	423	0.1	426	0.0	424	0.0	423	0.0
21	445	0.0	446	0.0	446	0.0	445	0.0
22	472	0.0	471	0.0	460	0.0	446	0.0
23	477	0.0	475	0.0	473	0.0	466	0.0
24	483	3.8	488	0.0	485	0.0	471	0.0
25	485	0.0	498	0.0	488	0.2	486	1.8
26	514	0.0	522	0.0	509	0.0	494	0.0
27	535	0.0	537	0.0	533	15.1	524	21.6
28	537	1.3	538	0.0	535	0.0	532	0.0
29	539	6.4	542	9.7	537	0.7	536	0.3
30	552	0.0	557	0.0	559	0.0	560	0.0
31	558	0.0	563	0.0	564	0.0	565	0.0
32	573	0.1	576	1.2	574	0.0	571	0.0
33	575	0.0	576	0.0	576	0.5	574	0.0
34	601	0.0	613	0.0	608	0.0	602	0.0
35	614	17.9	629	19.8	627	18.9	624	18.2
36	637	0.0	642	0.0	637	0.0	632	0.0
37	644	0.0	644	0.0	643	0.0	641	0.0
38	649	0.0	651	0.0	652	0.0	652	0.0
39	657	0.4	658	0.0	656	0.5	653	1.8
40	660	25.2	665	0.5	664	12.2	659	52.2
41	705	3.5	705	0.0	705	0.2	703	0.3
42	707	0.0	706	2.1	705	0.0	704	0.0
43	720	0.0	727	0.0	726	0.0	721	0.0
44	725	0.0	735	0.0	729	0.0	726	0.0
45	741	1.2	759	0.0	755	0.8	747	1.8
46	751	0.0	761	2.6	756	0.0	752	0.0
47	751	0.0	775	4.3	775	0.0	768	0.0
48	752	0.1	775	0.3	776	7.4	770	7.1
49	768	0.5	778	4.9	776	1.5	774	0.0
50	769	0.0	782	0.0	781	0.0	775	11.1
51	772	0.7	788	0.0	784	4.8	795	2.3
52	783	0.0	789	0.0	796	0.0	803	0.0

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Table 1 - continued from previous page

Numb. of the mode	Anion Freq. (cm^{-1})	Anion Int. (km mol^{-1})	Neutral Freq. (cm^{-1})	Neutral Int. (km mol^{-1})	Cation Freq. (cm^{-1})	Cation Int. (km mol^{-1})	Dication Freq. (cm^{-1})	Dication Int. (km mol^{-1})
53	789	0.0	807	0.0	820	0.0	836	0.0
54	797	0.0	820	0.0	835	0.0	850	0.0
55	798	10.4	843	73.8	856	97.1	855	0.0
56	818	0.0	852	0.0	865	0.0	870	135.0
57	831	0.0	868	0.0	866	0.0	879	0.0
58	836	194.4	882	0.0	885	0.0	885	0.0
59	863	0.0	892	0.0	892	0.0	886	0.0
60	882	0.0	894	126.1	911	0.0	914	2.3
61	887	0.0	898	0.0	913	2.5	944	0.0
62	908	0.4	912	3.9	915	112.6	948	85.1
63	916	0.0	954	0.0	970	4.5	969	15.9
64	917	0.0	956	0.0	975	0.0	990	0.0
65	922	0.0	967	2.4	978	0.0	997	0.0
66	924	0.0	970	0.0	984	0.0	998	0.0
67	936	0.0	972	0.2	988	0.0	1004	0.0
68	937	0.0	975	0.0	996	0.0	1013	0.0
69	962	6.5	978	0.0	998	0.0	1015	0.0
70	1031	0.0	1035	0.0	1043	0.0	1047	0.0
71	1047	0.8	1060	0.2	1057	0.0	1049	1.0
72	1055	0.1	1063	1.5	1067	7.8	1068	27.9
73	1102	0.0	1106	0.0	1114	0.0	1106	0.0
74	1134	0.0	1144	0.0	1152	0.0	1128	0.0
75	1136	0.0	1153	0.5	1153	0.0	1159	0.0
76	1151	0.6	1155	0.0	1163	9.2	1163	19.7
77	1152	35.4	1166	12.0	1165	0.6	1163	23.6
78	1160	0.0	1167	0.0	1171	0.0	1169	0.0
79	1177	6.5	1171	3.5	1189	80.3	1182	0.0
80	1190	0.0	1206	0.0	1196	0.0	1202	164.3
81	1213	0.2	1207	0.0	1216	15.5	1214	0.0
82	1216	0.0	1215	0.0	1223	0.0	1220	38.5
83	1220	12.6	1227	0.1	1225	18.1	1221	26.9
84	1221	0.0	1228	0.0	1226	0.0	1234	0.0
85	1221	19.2	1239	16.2	1235	134.3	1242	167.8
86	1236	0.0	1249	0.0	1244	0.0	1245	0.0
87	1259	60.0	1273	9.1	1267	17.9	1275	20.4
88	1283	21.6	1302	14.5	1293	24.7	1290	8.6
89	1304	612.8	1310	0.0	1319	0.0	1324	0.0
90	1305	0.0	1313	3.3	1320	0.0	1326	0.0
91	1313	0.0	1314	0.0	1332	292.6	1332	391.3
92	1332	0.0	1349	0.0	1352	0.0	1352	0.0
93	1347	0.0	1360	0.0	1366	3.1	1357	296.7
94	1348	143.2	1372	13.2	1368	0.0	1359	0.0
95	1351	0.0	1373	0.0	1374	55.5	1374	191.3
96	1351	33.2	1376	0.1	1376	0.0	1375	0.0
97	1363	1.0	1390	2.7	1376	31.7	1380	14.8
98	1385	0.0	1400	6.5	1398	0.0	1383	0.0
99	1395	22.8	1407	0.0	1409	7.1	1420	7.9
100	1398	0.0	1421	0.0	1425	93.2	1420	322.0
101	1410	17.4	1422	0.0	1425	0.0	1424	0.0
102	1412	0.0	1430	0.6	1425	0.0	1431	0.2
103	1428	0.0	1433	0.2	1438	0.4	1431	0.0
104	1430	0.5	1446	3.1	1442	2.6	1449	19.1
105	1451	0.0	1456	0.0	1458	0.0	1457	0.0
106	1456	60.2	1476	0.0	1474	0.0	1467	0.0

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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})
107	1459	0.0	1484	0.6	1479	7.8	1479	0.0
108	1481	0.0	1493	0.0	1484	0.0	1493	157.9
109	1485	0.0	1502	0.0	1494	0.0	1494	0.0
110	1502	7.0	1519	2.9	1503	10.3	1496	5.6
111	1517	0.0	1540	0.4	1532	86.0	1521	0.0
112	1524	3.2	1571	0.0	1538	0.0	1533	89.1
113	1545	123.1	1583	0.0	1546	87.8	1538	222.9
114	1560	0.0	1584	0.0	1556	0.0	1541	0.0
115	1575	51.8	1598	20.0	1574	225.3	1564	605.6
116	1580	95.9	1602	0.0	1584	0.0	1577	0.0
117	1583	0.0	1602	0.0	1584	3.8	1580	36.6
118	1590	0.0	1613	15.6	1597	0.0	1610	0.0
119	3011	4.9	3042	0.8	3063	4.6	3066	0.0
120	3011	0.0	3043	0.0	3063	0.0	3066	0.4
121	3013	0.0	3043	0.0	3067	0.0	3079	0.0
122	3014	72.7	3044	6.2	3067	3.0	3079	0.3
123	3015	12.8	3044	28.1	3068	0.4	3079	0.3
124	3015	0.0	3045	0.0	3068	0.0	3079	0.0
125	3024	0.0	3046	0.0	3069	0.0	3081	0.0
126	3024	27.8	3046	5.7	3069	0.2	3081	0.6
127	3036	72.7	3063	3.0	3084	0.0	3094	0.0
128	3036	0.0	3063	0.0	3084	0.0	3094	0.0
129	3039	0.0	3064	0.0	3085	0.0	3094	0.0
130	3040	346.9	3065	151.9	3085	36.3	3094	0.1
131	3040	334.5	3066	178.7	3086	65.2	3096	1.4
132	3042	0.0	3066	0.0	3086	0.0	3096	0.0