

Harmonic vibrational frequencies of circumbiphenyl ($C_{38}H_{16}$) 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	32	0.0	36	0.0	35	0.0	30	0.0
2	43	0.1	42	0.2	42	0.4	42	0.6
3	79	0.0	85	0.0	85	0.0	80	0.0
4	106	1.1	103	3.5	104	7.2	101	12.5
5	107	0.0	107	0.0	106	0.0	103	0.0
6	129	0.0	136	0.0	133	0.0	127	0.0
7	150	0.0	149	0.0	145	0.0	141	0.0
8	205	7.3	207	1.3	207	0.0	204	0.3
9	217	1.2	212	1.2	209	1.3	205	1.1
10	237	0.0	236	0.0	236	0.0	233	0.0
11	245	0.0	247	0.0	244	0.0	238	0.0
12	262	1.2	270	0.0	269	0.0	261	0.0
13	268	0.0	273	1.7	273	3.0	268	0.0
14	279	0.0	285	0.0	275	0.0	269	0.0
15	283	0.0	286	0.0	278	0.0	271	4.6
16	290	0.0	291	0.0	279	0.0	278	0.0
17	350	0.1	352	0.0	346	0.0	340	0.0
18	355	0.0	359	1.6	362	1.8	362	1.6
19	360	0.0	367	0.0	368	0.0	368	0.0
20	369	0.0	368	0.0	371	0.0	375	0.0
21	394	5.7	393	2.3	394	19.8	395	22.6
22	409	0.0	409	0.3	409	1.2	407	1.3
23	422	0.0	428	0.0	419	0.0	410	0.0
24	423	0.0	435	0.0	423	0.0	414	0.0
25	435	26.7	437	0.0	439	0.0	439	9.1
26	437	0.0	439	2.7	439	3.8	439	0.0
27	469	0.0	466	0.0	460	0.0	449	0.0
28	477	9.1	477	1.4	476	0.5	454	0.0
29	487	0.0	493	0.0	479	0.0	472	0.4
30	491	0.0	495	0.0	486	0.0	480	0.0
31	494	8.0	499	10.8	501	11.5	492	0.0
32	522	0.0	530	0.0	512	0.0	501	13.0
33	529	12.8	532	0.2	530	10.1	518	0.0
34	530	0.0	533	0.0	532	0.0	529	0.0
35	546	0.0	558	0.0	535	0.0	530	20.0
36	555	0.0	558	0.0	558	0.0	556	0.0
37	555	11.8	564	0.0	564	0.0	564	0.0
38	557	0.0	565	9.7	566	8.0	568	6.3
39	595	29.0	599	0.0	600	4.5	597	30.2
40	602	0.0	613	0.0	615	0.4	611	13.4
41	616	0.0	614	0.0	615	0.0	612	0.4
42	617	7.9	617	0.2	616	0.0	616	0.0
43	617	0.5	625	10.2	618	11.6	618	0.0
44	648	0.0	655	5.7	653	0.1	650	3.6
45	650	0.0	660	0.0	660	0.0	656	0.4
46	655	0.0	663	0.3	662	0.0	656	0.0
47	660	1.5	671	0.0	663	0.0	663	0.0
48	670	0.0	671	0.0	671	0.0	668	0.0
49	673	0.0	673	0.0	671	0.0	668	0.0
50	698	0.1	708	6.2	709	2.1	708	0.1
51	707	1.1	708	1.0	709	2.5	710	3.4
52	726	0.0	732	0.0	731	0.0	729	0.0

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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	731	0.0	745	0.0	742	0.0	737	0.0
54	739	0.0	750	0.0	743	0.0	742	0.0
55	743	0.0	754	0.0	751	0.0	745	0.0
56	754	0.0	760	0.0	761	0.0	760	0.0
57	759	0.0	773	0.0	778	1.3	771	3.6
58	764	20.7	774	0.0	778	5.1	773	0.0
59	773	1.6	782	11.8	784	0.0	777	0.0
60	780	0.0	797	0.0	785	0.0	777	6.1
61	783	0.0	798	0.0	788	0.0	795	0.0
62	786	0.3	801	0.0	798	0.0	802	0.0
63	787	0.0	806	10.7	818	10.4	825	36.0
64	798	0.0	814	0.0	826	0.0	833	6.0
65	808	0.0	828	16.2	827	7.5	842	0.0
66	810	0.0	831	0.0	846	0.0	843	1.7
67	824	5.5	832	0.0	846	0.0	860	0.0
68	825	0.0	849	6.2	846	2.7	862	0.0
69	828	201.8	852	0.0	866	0.0	869	0.0
70	844	1.5	855	205.9	868	227.1	879	0.0
71	869	0.0	876	0.0	875	0.0	881	246.2
72	894	0.0	945	0.0	948	0.0	946	0.0
73	897	0.0	949	0.0	954	68.6	952	134.3
74	912	0.0	949	0.0	961	0.0	974	0.0
75	912	0.0	954	0.0	966	0.0	976	0.0
76	929	0.0	956	0.0	970	0.0	982	0.0
77	930	0.0	961	1.5	974	0.0	983	0.0
78	944	0.0	964	0.0	976	2.6	990	4.1
79	944	0.4	969	0.0	983	0.0	993	0.0
80	945	0.0	971	0.0	986	0.0	1000	0.0
81	950	0.3	975	0.0	991	0.0	1002	0.0
82	969	3.6	976	0.2	994	0.0	1011	0.0
83	983	0.0	984	0.0	995	0.0	1011	0.1
84	1043	0.0	1050	0.0	1036	0.0	1036	0.0
85	1054	0.0	1065	0.0	1063	0.0	1059	0.0
86	1076	12.3	1082	3.0	1084	21.5	1081	96.2
87	1105	0.0	1130	1.4	1131	0.1	1126	5.9
88	1119	7.4	1148	0.0	1135	0.0	1137	0.0
89	1144	0.0	1161	0.0	1156	0.0	1156	0.0
90	1145	0.0	1161	4.2	1158	0.0	1158	0.0
91	1148	74.4	1166	0.5	1161	160.6	1159	171.4
92	1162	9.9	1167	0.0	1173	0.8	1170	1.3
93	1163	0.4	1175	0.2	1174	1.5	1171	90.4
94	1177	0.0	1184	1.3	1191	0.0	1205	0.0
95	1206	0.0	1204	1.4	1215	80.5	1207	0.0
96	1208	18.5	1210	0.0	1215	73.7	1218	0.1
97	1212	63.2	1214	0.0	1215	0.0	1223	176.2
98	1217	0.1	1224	0.0	1227	0.0	1237	0.0
99	1223	0.0	1229	3.5	1235	0.0	1238	0.0
100	1225	25.9	1229	5.0	1238	3.0	1239	135.8
101	1231	0.0	1236	0.0	1238	0.0	1245	0.0
102	1234	0.0	1243	0.0	1243	0.0	1246	4.6
103	1268	95.4	1261	18.1	1275	6.5	1279	0.1
104	1272	1.9	1282	17.5	1283	3.0	1293	1.5
105	1293	272.1	1297	29.1	1302	107.3	1298	0.0
106	1293	0.0	1311	0.0	1304	0.0	1309	37.1

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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})
107	1308	0.0	1329	0.0	1328	0.0	1321	320.0
108	1310	929.5	1331	0.0	1335	0.0	1330	0.0
109	1310	203.8	1337	0.0	1336	161.9	1339	0.0
110	1325	0.0	1344	1.2	1338	386.4	1345	686.0
111	1326	0.0	1352	9.3	1346	0.0	1352	0.0
112	1334	0.0	1363	0.0	1358	0.0	1356	0.0
113	1346	0.0	1376	2.4	1360	0.9	1362	29.9
114	1347	0.1	1386	0.2	1366	0.0	1363	0.0
115	1378	0.7	1387	0.0	1391	0.1	1384	0.0
116	1379	10.0	1393	0.0	1392	0.0	1395	0.1
117	1380	0.0	1395	1.3	1396	0.0	1397	0.0
118	1383	0.0	1399	0.0	1399	0.3	1401	0.1
119	1404	0.0	1422	0.0	1428	0.0	1426	0.0
120	1415	0.0	1426	2.2	1431	3.5	1432	19.2
121	1421	12.7	1428	1.3	1433	0.0	1433	0.0
122	1427	5.0	1442	1.0	1435	29.1	1440	22.7
123	1432	0.0	1446	0.0	1438	0.0	1441	0.0
124	1432	0.2	1453	0.0	1442	3.6	1448	147.9
125	1461	0.0	1467	0.0	1475	0.0	1467	4.9
126	1469	0.1	1474	5.4	1477	2.5	1470	14.0
127	1471	95.7	1483	7.5	1477	0.0	1475	0.0
128	1484	0.0	1506	1.2	1498	0.0	1489	0.0
129	1487	15.8	1514	0.0	1500	15.3	1503	69.1
130	1497	0.0	1515	0.0	1510	0.0	1515	0.0
131	1515	0.0	1539	0.6	1518	0.0	1532	0.0
132	1515	0.0	1539	0.0	1526	0.0	1536	0.0
133	1535	1.4	1545	0.4	1542	3.3	1544	444.6
134	1535	23.6	1587	0.0	1544	1.5	1548	25.0
135	1556	537.8	1590	0.0	1565	629.3	1556	0.0
136	1573	0.0	1599	13.2	1574	401.2	1560	574.4
137	1575	121.8	1604	0.0	1574	0.0	1565	0.0
138	1575	0.0	1605	0.0	1577	0.0	1572	802.8
139	1589	70.4	1605	17.3	1593	7.8	1587	31.8
140	1593	0.0	1606	5.5	1596	0.0	1593	0.0
141	3016	0.0	3044	0.0	3066	0.0	3078	0.0
142	3016	4.6	3044	4.2	3066	0.5	3078	0.2
143	3019	91.0	3046	4.9	3067	1.2	3079	0.1
144	3019	0.0	3046	0.0	3067	0.0	3079	0.0
145	3028	0.0	3051	0.0	3071	0.0	3080	0.0
146	3029	21.1	3051	9.4	3071	4.8	3081	1.4
147	3030	60.0	3052	52.4	3072	17.1	3081	0.1
148	3031	0.0	3052	0.0	3072	0.0	3081	0.0
149	3042	0.0	3065	0.0	3084	0.0	3094	0.0
150	3043	129.0	3065	54.9	3084	15.2	3094	0.4
151	3045	433.2	3067	194.6	3086	99.8	3096	10.7
152	3045	0.0	3067	0.0	3086	0.0	3096	0.0
153	3066	0.0	3086	0.0	3103	0.0	3107	0.0
154	3066	2.3	3086	1.0	3104	1.4	3107	0.0
155	3083	174.1	3105	89.3	3120	33.8	3124	4.4
156	3084	0.0	3105	0.0	3120	0.0	3124	0.0