

Harmonic vibrational frequencies of tetrabenzocoronene ($C_{36}H_{16}$) 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	31	0.0	29	0.0	35	0.0	36	0.0
2	55	0.3	53	0.6	55	1.1	53	2.1
3	66	0.0	60	0.0	70	0.0	74	0.0
4	98	0.6	98	2.4	96	5.3	95	9.5
5	122	0.0	124	0.0	124	0.0	123	0.0
6	134	0.0	127	0.0	136	0.0	140	0.0
7	155	0.0	154	0.0	151	0.0	147	0.0
8	208	0.0	206	0.0	211	0.5	211	1.9
9	208	0.2	209	0.0	212	0.0	213	0.0
10	232	26.6	233	12.1	230	29.4	234	0.2
11	263	0.0	269	0.0	271	3.6	262	4.2
12	273	0.0	274	0.0	271	0.0	273	0.0
13	280	0.0	278	2.6	276	0.0	273	0.0
14	288	1.8	281	0.0	277	0.0	279	0.0
15	294	0.0	292	0.1	291	2.1	287	2.8
16	304	0.0	305	0.0	305	0.0	303	0.0
17	311	0.0	311	0.0	310	0.0	307	0.0
18	313	0.0	322	0.0	331	0.0	337	0.0
19	336	0.0	342	0.0	354	0.0	349	0.0
20	371	0.0	362	0.0	356	0.0	364	0.0
21	389	0.0	388	0.0	391	0.0	392	0.0
22	397	0.0	402	0.0	402	0.0	401	0.0
23	408	0.9	409	1.1	407	0.1	405	0.0
24	431	6.0	433	1.5	434	1.9	434	6.0
25	447	0.0	447	0.0	448	0.0	448	0.0
26	497	0.0	498	0.0	491	0.1	484	0.3
27	498	0.0	501	0.0	494	0.0	492	0.0
28	505	0.0	504	0.0	502	0.0	497	0.0
29	520	0.0	505	0.0	506	0.0	500	0.6
30	523	1.4	519	0.9	512	0.0	505	0.0
31	530	0.0	522	4.1	520	15.6	516	39.1
32	533	4.6	531	0.0	529	0.0	526	0.0
33	539	2.7	538	11.3	533	17.5	528	25.9
34	548	0.0	545	0.0	544	0.0	540	0.0
35	563	11.8	564	5.5	562	30.3	558	0.0
36	572	0.0	569	0.0	565	0.0	564	5.9
37	592	25.7	595	3.4	594	0.7	593	8.7
38	610	0.0	610	0.0	603	0.0	599	0.0
39	611	0.0	610	0.0	611	0.0	610	0.0
40	626	0.0	627	10.9	625	40.0	627	6.9
41	626	32.1	629	0.0	628	0.0	627	0.0
42	634	0.0	632	0.0	635	0.0	634	0.0
43	635	0.0	638	0.0	636	0.0	635	0.0
44	637	0.0	639	0.0	637	0.0	636	0.0
45	638	0.0	640	0.0	643	0.0	643	0.0
46	652	43.0	651	17.0	652	32.5	653	0.2
47	694	0.0	707	0.0	702	13.2	695	17.6
48	703	12.4	708	12.1	711	0.0	711	0.0
49	721	4.6	726	0.4	726	0.0	726	1.9
50	729	0.0	747	0.0	746	0.0	741	0.0
51	734	0.0	748	0.0	755	0.0	758	50.1
52	748	0.0	764	80.3	761	55.4	759	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	751	101.3	765	1.1	765	0.0	762	0.0
54	757	0.0	766	0.0	767	2.7	767	6.7
55	758	18.6	769	0.0	779	0.0	780	0.0
56	765	0.0	775	0.0	783	0.0	788	0.0
57	766	0.0	780	0.0	784	0.0	796	0.0
58	766	16.5	781	50.7	789	93.5	798	109.6
59	774	0.0	796	0.0	810	0.0	818	0.3
60	792	0.0	814	0.0	820	0.0	821	0.0
61	800	0.0	821	1.1	820	0.3	827	0.0
62	814	0.0	842	0.0	852	0.0	854	0.0
63	818	13.7	847	0.0	868	0.0	902	0.0
64	830	0.0	848	0.0	870	0.0	902	0.0
65	832	67.8	879	0.0	905	0.0	908	0.0
66	842	0.0	880	65.1	906	45.5	926	0.0
67	851	0.0	889	0.0	909	0.0	929	0.2
68	853	0.0	895	0.0	919	0.0	933	0.0
69	860	0.0	903	0.0	924	0.0	935	17.4
70	862	68.9	904	44.8	924	0.0	948	0.0
71	905	0.0	909	0.0	930	32.4	951	0.0
72	915	0.0	919	0.0	933	0.0	971	0.0
73	928	51.2	931	13.7	934	38.7	971	43.2
74	941	0.0	974	0.0	987	5.2	988	2.0
75	942	0.0	975	0.0	995	0.0	1015	0.0
76	945	0.0	976	0.0	996	0.0	1016	0.0
77	945	3.6	977	3.0	998	0.0	1017	0.0
78	982	4.1	983	2.3	999	1.6	1018	0.7
79	1013	36.2	1013	1.9	1017	5.5	1019	0.0
80	1014	0.0	1015	0.0	1019	0.0	1020	6.2
81	1066	0.0	1067	0.0	1075	0.0	1079	0.0
82	1076	0.0	1074	0.0	1081	3.4	1079	36.2
83	1076	65.0	1077	6.9	1082	0.0	1085	0.0
84	1093	0.1	1095	0.8	1101	4.2	1103	0.0
85	1097	0.0	1097	0.0	1102	0.0	1105	1.5
86	1129	67.9	1133	16.5	1139	25.0	1142	7.7
87	1144	0.0	1150	0.0	1154	0.0	1156	0.0
88	1149	18.8	1154	1.5	1159	27.4	1163	103.4
89	1174	0.0	1174	0.0	1186	0.0	1196	0.0
90	1179	41.6	1183	1.1	1194	81.1	1201	105.6
91	1186	17.1	1189	1.4	1195	34.9	1204	6.8
92	1193	0.0	1196	0.0	1206	0.0	1212	0.0
93	1197	6.9	1199	1.5	1209	0.4	1215	4.1
94	1203	0.0	1204	0.0	1212	0.0	1223	0.0
95	1213	0.0	1216	0.0	1224	0.0	1230	0.0
96	1219	91.1	1230	0.0	1231	31.5	1239	20.0
97	1263	185.6	1273	0.0	1272	348.8	1271	554.3
98	1268	0.0	1281	5.1	1279	0.0	1277	0.0
99	1281	135.5	1283	0.0	1290	127.7	1287	0.0
100	1282	0.0	1289	59.5	1294	0.0	1295	0.2
101	1291	0.0	1293	0.4	1300	0.0	1314	0.0
102	1303	0.0	1300	0.0	1308	0.4	1323	0.0
103	1303	65.9	1315	0.0	1310	0.0	1324	7.1
104	1316	308.8	1327	5.7	1330	304.4	1332	507.6
105	1331	0.0	1341	0.0	1345	0.0	1348	212.0
106	1332	46.9	1343	0.0	1348	4.2	1352	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})
107	1339	2.7	1351	1.6	1351	0.0	1352	0.0
108	1340	0.0	1365	2.5	1352	4.8	1364	46.3
109	1357	0.0	1368	0.0	1370	0.0	1373	0.0
110	1357	90.5	1373	0.0	1374	35.7	1385	3.0
111	1363	0.0	1376	0.4	1384	12.9	1387	101.4
112	1373	1.1	1377	0.1	1384	52.0	1392	82.3
113	1375	7.8	1381	9.3	1386	0.0	1407	1.7
114	1386	57.9	1406	7.4	1406	0.4	1417	0.0
115	1407	0.0	1413	0.0	1421	0.0	1428	0.0
116	1427	2.0	1433	0.0	1436	0.3	1437	3.0
117	1428	0.0	1434	0.0	1439	0.0	1444	0.0
118	1438	0.0	1441	0.0	1448	0.0	1452	0.0
119	1459	113.3	1468	0.0	1468	0.0	1471	0.0
120	1461	0.0	1469	0.0	1471	0.0	1476	158.1
121	1465	0.0	1470	5.7	1474	5.1	1477	0.0
122	1481	15.9	1491	0.0	1487	68.7	1484	235.8
123	1484	364.6	1504	27.2	1499	0.1	1503	84.4
124	1515	83.7	1529	0.0	1525	44.9	1519	18.0
125	1532	0.0	1537	4.1	1533	0.0	1527	0.0
126	1536	0.0	1542	0.0	1541	0.0	1542	0.0
127	1540	39.5	1544	0.0	1543	3.9	1544	85.3
128	1540	0.0	1545	11.9	1551	0.0	1555	0.0
129	1547	0.0	1566	17.8	1555	165.3	1564	362.2
130	1549	454.9	1577	0.0	1558	0.0	1564	0.0
131	1569	0.0	1585	3.9	1574	0.3	1565	183.7
132	1573	0.0	1589	0.0	1577	0.0	1571	0.0
133	1574	0.0	1592	0.0	1579	0.0	1582	0.0
134	1577	283.0	1602	48.4	1586	0.4	1584	76.2
135	3022	0.0	3046	0.0	3062	0.0	3066	0.0
136	3022	54.3	3046	2.7	3062	0.6	3066	0.3
137	3022	76.0	3049	21.1	3065	1.5	3068	0.0
138	3023	0.0	3049	0.0	3065	0.0	3068	0.0
139	3026	0.0	3051	0.0	3072	0.0	3082	0.0
140	3026	25.5	3051	5.0	3072	0.4	3082	0.2
141	3030	72.3	3052	12.2	3072	0.0	3082	0.1
142	3031	0.0	3052	0.0	3072	0.0	3082	0.0
143	3045	0.0	3067	0.0	3085	0.0	3092	0.7
144	3046	404.3	3067	142.4	3085	45.9	3092	0.0
145	3047	154.2	3070	66.5	3090	23.1	3100	0.4
146	3047	0.0	3070	0.0	3090	0.0	3100	0.0
147	3074	24.6	3083	0.0	3100	0.0	3107	0.0
148	3074	0.0	3083	31.9	3100	14.1	3107	0.0
149	3091	141.6	3097	102.6	3111	47.8	3115	5.2
150	3091	0.0	3097	0.0	3111	0.0	3115	0.0