

Harmonic vibrational frequencies of dicoronylene ( $C_{48}H_{20}$ ) 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	16	0.0	6	0.0	19	0.0	19	0.0
2	23	0.0	23	0.2	23	0.4	22	0.8
3	56	0.0	56	0.0	57	0.0	55	0.0
4	91	0.0	90	0.0	90	0.0	89	0.0
5	94	0.5	93	0.1	94	0.4	93	0.7
6	98	1.0	97	1.6	97	2.1	95	2.7
7	104	0.0	102	0.0	105	0.0	106	0.0
8	116	0.0	110	0.0	112	0.0	112	0.0
9	140	2.7	138	4.9	136	8.9	133	13.4
10	167	0.0	171	0.0	168	0.0	164	0.0
11	177	0.0	176	0.0	178	0.0	176	0.0
12	178	0.0	178	0.0	179	0.0	180	0.0
13	197	0.0	198	0.0	201	0.0	201	0.0
14	218	0.0	219	0.0	221	0.0	222	0.0
15	239	0.0	235	0.0	232	0.0	227	0.0
16	270	0.0	265	0.0	260	0.0	253	0.0
17	277	0.0	286	0.0	286	0.0	285	0.0
18	280	0.0	287	0.0	289	0.0	288	0.0
19	296	0.0	289	0.0	294	0.0	290	0.9
20	300	1.2	298	0.3	296	0.5	298	0.0
21	313	0.0	315	0.9	311	0.5	305	0.0
22	316	0.4	318	0.0	311	0.0	305	0.2
23	335	0.0	346	0.0	340	0.0	333	0.0
24	362	8.3	366	4.7	363	0.0	362	0.0
25	365	0.0	366	0.0	365	32.9	364	39.0
26	369	6.0	371	0.9	368	0.0	366	1.3
27	379	0.0	381	0.0	379	0.0	372	0.0
28	388	0.0	394	0.0	383	0.0	377	0.0
29	397	24.8	400	4.0	398	0.3	397	0.0
30	413	0.0	414	2.9	414	4.1	411	6.8
31	415	1.2	416	0.0	416	0.0	415	0.0
32	443	0.0	442	0.0	443	0.0	439	0.6
33	450	0.2	448	0.0	444	0.2	444	0.0
34	457	0.0	454	0.0	456	0.0	453	0.0
35	463	0.0	466	0.0	461	0.0	456	0.0
36	470	39.6	472	3.7	473	0.4	467	0.0
37	476	0.0	477	0.0	474	0.0	471	0.0
38	487	0.0	491	0.0	480	0.0	473	5.1
39	498	0.4	499	0.1	499	1.7	498	3.8
40	510	0.0	511	0.0	511	0.0	511	0.0
41	516	0.0	530	1.8	527	4.2	522	0.0
42	527	6.8	531	0.5	528	0.0	523	7.3
43	527	7.6	534	0.0	530	4.1	528	2.9
44	528	0.0	534	0.0	533	0.0	530	10.7
45	530	0.0	536	0.0	534	0.0	533	0.0
46	534	20.7	540	0.0	536	17.4	534	0.0
47	537	0.0	542	20.7	541	0.0	543	0.0
48	545	0.0	547	0.0	548	0.0	546	0.0
49	560	0.0	557	0.0	559	0.0	559	0.0
50	573	14.3	573	18.8	568	26.5	564	36.4
51	597	0.0	598	0.0	592	0.0	585	0.0
52	610	3.6	614	0.6	610	9.5	606	18.4

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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	622	0.0	621	0.0	622	0.0	622	0.0
54	624	0.0	635	0.1	633	0.1	631	0.2
55	626	0.0	635	0.0	635	0.0	633	0.0
56	630	0.0	636	0.0	636	0.0	635	0.0
57	640	0.0	642	0.0	639	0.0	638	0.0
58	642	0.0	648	0.1	645	0.4	641	0.6
59	643	0.0	649	0.0	652	0.0	651	0.0
60	647	0.0	655	0.0	657	0.0	668	0.0
61	676	1.9	677	0.2	675	1.1	674	0.0
62	679	1.2	681	0.0	680	0.8	677	0.6
63	681	0.0	683	1.1	680	0.0	679	0.0
64	691	0.0	690	0.0	691	0.0	691	0.0
65	714	0.0	715	0.0	716	0.0	714	0.0
66	715	0.0	722	0.0	718	0.0	714	0.0
67	732	0.2	736	4.4	736	5.5	734	5.3
68	735	1.7	738	2.5	738	1.9	735	12.3
69	744	0.0	755	0.0	750	1.7	746	1.9
70	745	0.0	755	1.3	757	0.0	758	0.0
71	751	0.6	757	0.0	759	0.0	760	0.0
72	760	0.0	775	0.0	771	0.0	771	0.0
73	761	0.0	779	0.0	780	0.9	774	0.2
74	764	0.0	780	0.0	780	0.0	774	0.0
75	776	1.5	783	0.0	781	0.0	778	0.0
76	778	0.0	785	0.0	784	0.0	783	52.8
77	780	0.0	786	1.6	784	0.0	790	0.0
78	790	0.0	792	0.0	791	0.0	790	0.0
79	794	1.6	797	26.2	796	13.9	791	0.0
80	796	1.1	805	4.5	798	20.3	792	0.0
81	797	0.0	806	0.0	800	0.0	797	15.3
82	798	5.0	807	0.9	806	9.0	807	14.1
83	798	0.0	808	0.0	810	0.0	808	1.4
84	800	0.0	811	0.1	810	2.4	812	0.0
85	802	0.0	827	0.0	837	0.0	848	0.0
86	806	7.6	827	0.0	837	0.0	848	0.0
87	829	74.9	852	126.1	863	116.4	875	110.9
88	830	0.0	852	0.0	864	0.0	876	0.0
89	837	0.0	877	0.0	888	0.0	902	0.0
90	850	0.0	885	0.0	894	0.0	904	0.3
91	852	0.0	889	0.0	899	0.0	905	0.0
92	858	204.6	894	158.9	900	179.1	906	0.0
93	897	0.0	897	0.0	903	0.0	909	196.8
94	902	0.8	904	1.4	905	0.5	912	0.0
95	927	0.0	940	0.0	939	0.0	937	0.0
96	927	0.0	954	0.0	969	0.0	981	0.0
97	935	0.0	955	0.0	969	0.0	982	0.0
98	935	0.8	962	0.0	978	0.0	984	1.2
99	936	0.0	963	0.1	978	0.0	988	0.0
100	951	0.0	970	0.0	986	0.0	992	0.0
101	951	0.0	970	0.0	986	0.0	992	0.2
102	953	0.0	976	0.0	991	0.3	999	0.1
103	953	0.0	976	0.0	993	0.0	1000	0.0
104	986	5.4	995	0.0	993	0.0	1000	0.0
105	989	0.0	996	0.0	993	0.1	1008	0.0
106	992	8.7	998	12.7	1000	1.1	1008	0.5

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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	1024	0.0	1029	0.0	1031	0.0	1032	0.0
108	1033	0.9	1038	0.2	1040	63.5	1035	30.2
109	1046	0.2	1053	0.4	1049	11.5	1041	182.4
110	1091	0.0	1092	0.0	1100	0.0	1104	0.0
111	1139	0.0	1147	0.0	1151	0.0	1151	0.0
112	1141	3.2	1151	13.9	1153	11.0	1153	7.3
113	1143	70.0	1152	2.0	1154	1.2	1154	21.5
114	1148	0.0	1157	0.0	1158	0.0	1155	0.0
115	1153	0.0	1160	0.0	1161	0.0	1157	0.0
116	1153	10.7	1160	0.1	1161	4.3	1159	2.8
117	1164	3.3	1168	0.7	1169	7.4	1165	0.0
118	1169	0.0	1179	0.0	1177	0.0	1166	1.5
119	1176	0.0	1185	0.0	1184	0.0	1182	0.0
120	1181	150.3	1191	0.0	1188	213.5	1189	311.9
121	1196	26.6	1194	0.0	1202	0.0	1215	143.7
122	1199	0.0	1196	0.2	1204	47.1	1217	0.0
123	1211	106.7	1219	0.0	1218	289.3	1219	394.0
124	1212	0.0	1220	5.8	1220	0.0	1221	0.0
125	1218	83.4	1223	0.0	1228	0.0	1225	135.8
126	1223	0.0	1227	2.0	1229	33.2	1232	0.0
127	1228	8.4	1231	0.2	1237	69.4	1238	28.4
128	1232	149.6	1233	0.0	1240	15.5	1240	0.0
129	1236	0.0	1239	0.0	1241	0.0	1246	0.0
130	1238	0.0	1246	11.4	1245	0.0	1248	3.7
131	1255	0.0	1253	0.0	1264	0.0	1272	0.0
132	1283	100.4	1280	2.0	1297	3.8	1284	0.0
133	1291	67.9	1294	17.9	1304	74.0	1298	1.2
134	1299	0.0	1305	0.0	1306	0.0	1311	0.0
135	1301	0.0	1309	60.1	1308	0.0	1320	105.8
136	1306	447.0	1327	0.0	1318	49.3	1322	62.5
137	1313	808.4	1333	0.0	1331	787.2	1336	998.9
138	1331	0.0	1334	14.1	1344	0.0	1351	67.7
139	1331	0.0	1338	0.0	1344	0.0	1351	0.0
140	1338	26.0	1345	8.0	1345	17.1	1361	0.0
141	1352	53.7	1353	0.0	1370	13.6	1365	482.8
142	1353	127.7	1368	3.7	1371	0.0	1367	113.5
143	1360	0.0	1379	3.1	1371	87.8	1375	0.0
144	1366	0.0	1381	0.0	1378	0.0	1377	35.0
145	1369	18.8	1388	0.0	1380	0.1	1385	0.0
146	1374	0.0	1389	0.4	1388	0.0	1389	0.0
147	1378	5.9	1390	12.4	1391	1.2	1391	0.0
148	1382	0.0	1396	0.0	1392	0.0	1393	5.1
149	1398	0.0	1401	0.0	1411	0.0	1403	0.0
150	1402	0.1	1406	21.3	1412	17.0	1416	5.3
151	1407	0.0	1421	0.0	1412	0.0	1418	1.5
152	1412	16.6	1423	0.0	1420	7.1	1419	0.0
153	1427	5.4	1428	0.0	1432	37.2	1430	0.0
154	1430	18.0	1433	0.0	1436	0.0	1434	32.3
155	1431	0.0	1441	18.5	1438	0.0	1434	6.7
156	1432	0.0	1443	0.0	1439	12.2	1444	0.0
157	1444	118.4	1443	0.0	1449	106.0	1462	297.2
158	1448	2.9	1447	0.1	1456	0.0	1464	64.4
159	1450	0.0	1461	0.8	1460	6.6	1466	0.0
160	1451	0.0	1470	0.0	1467	0.0	1468	0.0

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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. ( $\text{km mol}^{-1}$ )
161	1461	43.2	1487	5.1	1476	2.2	1470	9.4
162	1475	0.6	1489	0.0	1478	0.1	1477	1.6
163	1485	0.0	1493	5.3	1487	0.0	1494	0.0
164	1498	0.0	1495	0.0	1500	0.0	1502	3.4
165	1511	6.7	1518	0.0	1517	4.0	1506	0.0
166	1513	0.0	1528	0.0	1519	0.2	1509	0.0
167	1516	25.4	1532	0.6	1522	0.0	1520	34.6
168	1528	0.0	1533	0.0	1528	0.0	1533	0.0
169	1548	97.2	1570	0.0	1553	0.0	1545	0.0
170	1551	0.0	1589	1.6	1560	42.6	1552	115.0
171	1561	0.0	1589	1.0	1564	0.0	1563	861.9
172	1572	570.7	1593	0.0	1567	718.4	1563	0.0
173	1582	776.4	1595	0.0	1583	762.3	1574	0.0
174	1585	0.0	1599	0.4	1583	0.0	1577	674.2
175	1590	42.8	1601	0.0	1592	246.6	1589	3.1
176	1592	0.0	1602	20.0	1593	4.0	1592	0.0
177	1594	514.9	1602	0.0	1595	0.0	1597	1314.6
178	1595	0.0	1604	82.9	1597	0.0	1605	0.0
179	3021	0.0	3043	0.0	3061	0.0	3073	0.0
180	3021	6.0	3043	5.1	3061	1.5	3073	0.6
181	3022	6.3	3044	12.2	3061	0.8	3073	1.3
182	3022	0.0	3044	0.0	3061	0.0	3073	0.0
183	3024	53.5	3045	0.0	3063	0.0	3074	0.1
184	3024	0.0	3045	3.7	3063	0.9	3074	0.0
185	3025	45.5	3046	2.2	3064	0.0	3075	0.0
186	3025	0.0	3046	0.0	3064	0.0	3075	0.0
187	3045	0.0	3063	0.0	3079	0.0	3089	0.0
188	3045	0.8	3063	1.6	3079	7.7	3089	1.1
189	3046	0.7	3064	3.8	3079	0.0	3089	0.2
190	3047	0.0	3064	0.0	3079	0.0	3089	0.0
191	3047	0.0	3065	0.0	3081	0.0	3091	0.0
192	3047	366.7	3065	199.5	3081	85.2	3091	20.8
193	3050	513.3	3066	262.5	3082	182.1	3091	41.7
194	3050	0.0	3067	0.0	3082	0.0	3091	0.0
195	3063	0.0	3069	0.0	3088	0.9	3094	10.0
196	3063	1.4	3069	2.7	3088	0.0	3094	0.0
197	3081	53.1	3088	36.1	3106	18.7	3114	6.5
198	3082	0.0	3088	0.0	3106	0.0	3115	0.0