

Harmonic vibrational frequencies of coronene (C<sub>24</sub>H<sub>12</sub>) 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 <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )
1	84	0.0	88	0.0	85	0.1	85	0.0
2	88	0.1	88	0.0	87	0.0	85	0.0
3	129	1.7	123	4.9	88	0.0	119	18.8
4	151	0.0	163	0.0	120	10.5	154	0.0
5	154	0.0	224	0.0	158	0.0	210	0.0
6	226	0.0	291	0.0	218	0.0	277	0.0
7	272	0.0	291	0.0	275	0.0	277	0.0
8	277	0.1	297	0.0	289	0.2	284	0.0
9	291	0.0	297	0.0	290	0.0	285	0.0
10	302	0.0	364	0.0	292	0.0	365	0.0
11	362	0.0	364	0.0	365	0.0	365	0.0
12	372	32.4	378	3.2	374	0.1	372	0.1
13	379	8.0	378	3.2	379	6.6	373	0.1
14	424	0.0	448	0.0	431	0.0	417	0.0
15	424	0.0	448	0.0	435	0.0	418	0.0
16	451	0.0	469	0.0	465	1.9	455	0.0
17	466	0.0	476	0.0	469	0.0	469	0.0
18	469	4.6	491	0.0	471	0.0	470	0.0
19	488	0.0	491	0.0	491	0.0	491	0.0
20	497	0.0	523	0.0	494	0.0	491	0.0
21	521	7.9	541	0.0	515	1.3	510	0.0
22	535	0.1	541	0.0	539	0.0	510	0.0
23	539	17.2	549	28.2	548	1.1	541	0.0
24	543	1.6	553	0.0	550	29.6	552	33.4
25	564	0.0	635	0.0	625	0.0	621	0.0
26	616	0.0	642	0.0	636	0.0	629	0.0
27	630	0.0	658	0.0	652	0.0	646	0.0
28	639	0.0	658	0.0	654	0.0	646	0.0
29	652	0.0	669	0.0	666	1.0	664	0.0
30	666	7.0	680	0.0	671	0.0	676	0.0
31	680	0.0	680	0.0	677	0.0	676	0.0
32	682	0.0	758	0.0	733	0.0	742	0.0
33	725	0.0	758	0.0	742	0.0	743	0.0
34	731	0.5	763	0.0	760	0.0	756	14.7
35	738	0.2	775	5.9	763	13.7	756	14.8
36	759	10.4	775	5.9	768	0.3	762	0.0
37	762	1.4	799	0.0	777	0.0	786	13.4
38	767	5.3	802	0.1	781	0.0	786	13.5
39	779	0.0	802	0.1	784	32.3	788	0.0
40	779	16.4	806	0.0	805	6.0	818	0.0
41	781	0.0	806	0.0	806	1.1	819	0.0
42	794	6.3	843	0.0	820	0.0	867	0.0
43	795	0.0	843	0.0	856	0.0	867	0.0
44	800	0.0	864	175.7	860	0.0	892	197.1
45	812	164.3	929	0.0	881	190.5	926	0.0
46	871	0.1	951	0.0	928	0.0	977	0.0
47	873	0.0	960	0.0	967	0.0	980	0.0
48	910	0.0	960	0.0	975	0.0	980	0.0
49	911	0.2	972	0.0	981	0.0	990	0.0
50	920	0.0	972	0.0	987	0.0	990	0.0
51	929	1.8	979	0.0	990	0.9	1005	0.0
52	931	0.0	986	0.0	996	0.0	1006	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. ( $\text{km mol}^{-1}$ )
53	971	0.0	986	0.0	997	0.0	1013	0.0
54	981	0.0	1021	0.0	1000	0.0	1036	0.0
55	1010	0.0	1140	6.5	1028	0.0	1126	46.8
56	1113	56.3	1140	6.5	1135	11.5	1127	47.0
57	1123	4.0	1156	0.0	1143	4.3	1132	0.0
58	1132	8.2	1165	0.0	1147	37.9	1159	0.0
59	1139	0.0	1167	0.0	1163	0.4	1159	0.0
60	1156	4.1	1167	0.0	1169	0.0	1167	0.0
61	1168	0.0	1182	0.0	1171	0.0	1205	0.8
62	1192	21.5	1214	1.0	1212	0.8	1205	0.8
63	1200	0.0	1214	1.0	1213	89.3	1229	0.0
64	1212	21.4	1223	0.0	1222	0.0	1230	0.0
65	1219	86.4	1225	0.0	1223	0.7	1237	0.0
66	1227	0.0	1225	0.0	1243	0.0	1237	0.0
67	1236	0.0	1245	0.0	1246	0.0	1244	0.0
68	1291	337.8	1312	24.0	1297	0.0	1295	182.1
69	1294	0.0	1312	24.0	1311	38.3	1296	181.7
70	1299	35.2	1336	0.0	1320	1.8	1353	511.2
71	1315	38.1	1343	0.0	1350	0.0	1353	510.7
72	1331	0.0	1387	0.8	1353	300.0	1358	0.0
73	1333	2.7	1387	0.8	1354	53.5	1358	0.0
74	1356	114.4	1390	0.0	1382	45.2	1391	0.0
75	1373	0.0	1390	0.0	1391	0.0	1391	0.0
76	1377	0.0	1422	0.0	1398	0.0	1430	0.0
77	1412	0.0	1424	0.0	1424	1.5	1431	0.0
78	1413	7.1	1424	0.0	1429	0.0	1431	0.0
79	1427	0.0	1445	0.0	1446	0.0	1455	0.0
80	1431	26.6	1445	0.0	1458	0.2	1456	0.0
81	1440	0.0	1474	0.0	1461	0.0	1457	0.0
82	1465	103.3	1494	1.3	1473	4.3	1457	0.0
83	1471	0.0	1494	1.3	1480	0.0	1472	20.0
84	1480	9.1	1529	0.0	1503	17.1	1472	17.5
85	1505	32.7	1530	0.0	1505	38.3	1478	288.0
86	1526	0.0	1591	0.0	1526	0.0	1478	286.3
87	1555	175.7	1599	0.0	1553	453.6	1506	0.0
88	1563	0.0	1599	0.0	1565	0.0	1524	0.0
89	1566	92.3	1602	13.1	1580	4.4	1597	0.0
90	1586	0.0	1602	13.1	1613	0.0	1598	0.0
91	3001	0.0	3042	0.0	3070	0.0	3083	0.0
92	3001	3.4	3043	8.1	3071	0.1	3083	1.8
93	3005	131.8	3043	8.1	3071	1.4	3084	1.8
94	3005	0.0	3045	0.0	3072	0.0	3085	0.0
95	3008	0.0	3045	0.0	3072	0.0	3085	0.0
96	3010	8.6	3045	0.0	3073	0.7	3085	0.0
97	3030	0.9	3062	0.0	3086	1.0	3095	0.1
98	3031	0.0	3063	0.0	3087	0.0	3096	0.0
99	3031	0.0	3063	0.0	3087	0.0	3096	0.0
100	3034	320.0	3065	139.9	3088	24.4	3097	4.4
101	3036	322.9	3065	139.9	3089	30.0	3097	4.5
102	3038	0.0	3067	0.0	3090	0.0	3098	0.0