

Harmonic vibrational frequencies of corannulene (C<sub>20</sub>H<sub>10</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	29	2.5	138	0.0	39	114.6	81	185.6
2	133	1.9	138	0.0	131	3.3	126	0.7
3	141	1.1	143	5.3	143	5.4	139	16.3
4	202	1.6	274	0.0	185	90.3	158	225.2
5	276	0.4	274	0.0	261	2.2	226	52.5
6	277	0.9	305	0.1	266	33.1	235	17.4
7	284	0.3	305	0.1	288	21.6	277	14.3
8	300	0.4	402	2.4	300	2.8	296	0.0
9	391	24.5	402	2.4	380	71.9	338	6.5
10	398	7.9	434	0.0	399	17.3	341	103.4
11	406	0.4	434	0.0	402	30.4	389	1.3
12	427	0.0	443	3.4	422	0.1	396	2.4
13	445	3.2	443	3.4	440	0.1	412	3.0
14	458	0.2	532	0.0	489	20.6	455	17.3
15	509	0.0	539	0.0	520	4.0	496	2.6
16	537	2.4	539	0.0	524	18.0	498	6.6
17	537	1.1	544	15.9	538	0.9	527	18.7
18	541	9.4	584	1.7	545	2.7	539	11.7
19	574	1.5	600	0.0	566	23.1	546	9.2
20	584	0.4	600	0.0	579	3.2	576	48.2
21	621	2.9	634	0.0	594	1.2	577	6.0
22	628	1.1	634	0.0	616	32.5	605	12.4
23	628	10.6	646	0.0	626	18.9	607	119.3
24	640	0.0	659	17.3	637	10.4	629	15.8
25	649	2.4	659	17.3	640	0.1	630	6.7
26	666	0.3	747	3.0	735	35.6	683	608.2
27	712	7.8	747	3.0	738	17.7	731	18.5
28	732	0.4	754	0.0	752	1.5	745	97.6
29	739	29.1	754	0.0	762	1.7	749	6.0
30	757	40.3	791	0.0	783	7.7	749	10.0
31	761	3.2	791	0.0	787	5.2	782	9.7
32	770	0.5	820	6.0	833	72.6	786	1.7
33	772	9.6	820	6.0	835	47.1	820	119.8
34	787	107.9	843	129.9	837	0.0	837	0.2
35	811	0.7	845	0.1	852	1.3	854	2.8
36	830	5.1	845	0.1	875	135.6	880	141.2
37	835	9.1	928	0.0	923	34.3	887	421.3
38	852	0.1	950	0.0	931	13.1	918	272.8
39	876	1.0	958	0.8	967	0.0	923	14.1
40	877	2.1	958	0.8	973	10.9	961	0.1
41	924	0.0	967	0.0	977	8.6	974	7.7
42	926	2.4	967	0.0	988	0.4	987	6.1
43	927	0.1	1020	1.6	988	3.7	988	26.1
44	1003	2.3	1068	0.0	1002	221.0	1000	0.7
45	1068	29.8	1068	0.0	1068	397.6	1016	8.8
46	1086	40.6	1138	0.0	1076	493.3	1023	94.2
47	1088	11.7	1138	0.0	1079	3.5	1068	44.2
48	1101	18.7	1146	4.3	1141	0.3	1075	51.0
49	1116	45.1	1146	4.3	1147	4.0	1101	249.2
50	1128	2.4	1165	0.0	1153	116.0	1149	5.7
51	1170	10.5	1165	0.0	1155	140.6	1151	78.3
52	1179	42.3	1187	0.0	1179	46.2	1167	1.2

continued on next page

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	1187	24.8	1187	0.0	1179	4.4	1177	52.1
54	1213	0.7	1220	0.0	1209	14.5	1213	73.5
55	1233	12.3	1239	1.4	1233	0.4	1225	81.4
56	1254	5.2	1304	9.8	1243	67.1	1235	6.3
57	1275	162.0	1304	9.8	1256	106.1	1258	171.6
58	1292	30.3	1338	0.0	1268	193.3	1275	38.8
59	1322	1.1	1338	0.0	1301	47.9	1287	6.1
60	1347	15.7	1399	2.8	1327	55.4	1319	185.6
61	1349	58.5	1399	2.8	1366	16.9	1324	18.9
62	1389	1.8	1401	0.0	1396	119.4	1369	302.2
63	1389	5.5	1401	0.0	1406	0.3	1380	24.9
64	1409	3.1	1423	2.1	1408	3.3	1397	3.8
65	1412	0.9	1436	0.0	1411	17.0	1405	32.1
66	1421	11.4	1436	0.0	1426	0.8	1429	19.2
67	1427	37.3	1437	2.9	1440	3.6	1430	12.5
68	1432	5.6	1437	2.9	1451	1.0	1443	0.2
69	1467	0.1	1469	0.0	1482	0.0	1456	29.5
70	1503	1.5	1599	1.5	1519	184.0	1482	18.1
71	1542	60.6	1599	1.5	1528	5.6	1515	46.9
72	1552	40.3	1603	0.0	1552	191.1	1541	42.1
73	1576	5.4	1603	0.0	1584	33.3	1566	20.8
74	1584	10.9	1608	0.0	1594	2.3	1568	38.0
75	2991	9.7	3041	0.0	3072	1.0	3081	3.9
76	2992	9.7	3041	7.0	3072	0.5	3082	1.1
77	2995	71.9	3041	7.0	3072	1.4	3082	6.3
78	2996	2.6	3042	0.0	3075	0.0	3088	0.5
79	2999	16.1	3042	0.0	3075	0.2	3088	1.1
80	3018	172.6	3060	0.0	3085	2.3	3092	10.8
81	3018	10.9	3060	0.0	3086	2.1	3092	17.2
82	3021	141.0	3061	115.5	3087	10.0	3093	8.2
83	3023	283.6	3061	115.5	3089	17.9	3100	10.2
84	3026	29.0	3063	6.3	3090	2.1	3100	2.5