Harmonic vibrational frequencies of dibenzo[bc,kl]coronene ($C_{30}H_{14}$) 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	48	0.0	46	0.2	47	1.3	48	3.4
2	82	0.0	83	0.0	83	0.0	81	0.0
3	117	1.7	114	4.2	112	7.2	109	11.2
4	120	0.0	117	0.0	117	0.0	116	0.0
5	138	0.0	139	0.0	140	0.0	138	0.0
6	221	0.8	217	0.2	216	0.0	213	0.1
7	224	0.0	234	0.0	231	0.0	229	0.0
8	238	11.4	243	1.2	242	2.3	240	3.4
9	261	0.0	261	0.0	253	0.0	245	0.0
10	266	0.0	267	0.0	270	0.0	271	0.0
11	295	0.0	295	0.0	296	0.0	296	0.0
12	310	0.0	319	0.0	321	1.5	313	4.3
13	324	0.1	329	0.2	327	0.0	332	0.0
14	340	0.0	341	0.0	339	0.0	335	0.0
15	351	0.0	343	0.0	340	0.0	338	0.0
16	373	0.0	376	0.0	375	0.0	375	0.0
17	389	0.0	389	0.0	393	0.0	397	0.0
18	401	8.7	399	7.0	401	6.6	403	4.3
19	426	2.2	425	2.6	425	0.1	423	0.1
20	432	0.0	431	0.0	434	0.0	435	0.0
21	449	0.0	463	0.0	454	0.0	446	0.0
22	482	12.9	486	1.6	486	0.1	483	3.5
23	486	0.0	487	0.0	486	0.0	484	0.0
24	505	6.5	508	3.3	499	0.0	487	24.0
25	528	0.0	531	0.0	534	0.0	527	0.0
26	542	6.6	540	14.6	536	26.3	535	34.7
27	547	0.0	549	0.0	538	0.0	535	0.0
28	555	0.5	555	1.9	553	0.0	550	1.3
29	565	0.0	564	0.0	559	0.0	552	0.0
30	567	0.0	566	0.0	564	0.0	563	0.0
31	599	0.0	608	0.0	598	0.0	590	0.0
32	617	3.4	617	2.3	617	7.0	616	13.1
33	622	0.0	624	0.0	621	0.0	616	0.0
34	622	0.0	627	0.0	628	0.0	628	0.0
35	634	0.0	638	0.0	635	0.0	633	0.0
36	644	0.0	650	0.0	650	0.0	650	4.8
37	646	6.4	652	0.5	652	0.7	650	0.0
38	656	0.0	656	0.0	656	0.0	656	0.0
39	671	3.5	672	0.7	666	2.9	660	5.0
40	712	0.0	718	6.1	722	0.8	722	0.0
41	716	11.5	734	0.0	727	0.0	723	3.8
42	722	61.2	754	0.0	754	60.7	756	47.4
43	745	0.0	754	71.5	762	0.0	770	0.0
44	757	0.0	769	0.0	778	0.0	781	0.0
45	764	0.0	782	2.5	785	0.0	785	26.2
46	773	2.0	783	1.7	786	2.5	798	0.0
47	778	0.0	785	0.6	788	21.8	800	41.7
48	782	0.0	787	0.0	794	2.4	800	10.8
49	783	3.2	790	0.0	797	0.0	809	0.0
50	787	0.0	790	0.0	804	0.0	817	0.0
51	792	0.1	810	0.0	818	0.5	828	1.7
52	797	0.4	858	0.0	873	2.2	871	1.3

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Table 1 - continued from previous page

Numb. of the mode	Anion Freq. (cm^{-1})	Anion Int. (km mol^{-1})	Neutral Freq. (cm^{-1})	Neutral Int. (km mol^{-1})	Cation Freq. (cm^{-1})	Cation Int. (km mol^{-1})	Dication Freq. (cm^{-1})	Dication Int. (km mol^{-1})
53	803	0.0	870	0.0	880	0.0	878	0.0
54	839	0.0	872	3.8	885	0.0	902	0.0
55	845	0.0	881	0.0	896	0.0	915	0.0
56	852	0.0	886	0.0	901	0.0	926	0.0
57	855	165.8	897	148.4	905	0.0	927	0.0
58	870	9.8	900	0.0	916	134.0	939	114.7
59	876	0.0	906	0.0	937	0.0	980	0.0
60	892	0.0	911	0.0	941	0.0	983	0.0
61	936	0.0	974	0.0	987	0.0	990	0.0
62	936	1.6	976	4.2	990	0.0	1001	0.0
63	945	0.0	976	0.0	990	0.0	1003	0.0
64	946	0.0	978	0.0	1000	1.1	1027	0.1
65	983	0.0	980	0.0	1001	0.0	1028	0.0
66	1033	18.6	1037	2.0	1040	1.3	1040	35.5
67	1034	3.1	1043	1.7	1044	9.6	1047	4.9
68	1046	0.0	1050	0.0	1056	0.0	1058	0.0
69	1071	0.0	1074	0.0	1079	0.0	1081	0.0
70	1072	0.0	1075	0.0	1082	0.0	1087	0.0
71	1103	0.1	1111	2.3	1115	8.7	1118	35.1
72	1145	12.0	1148	3.6	1157	5.3	1163	44.3
73	1166	11.3	1167	2.6	1177	1.8	1182	46.6
74	1167	0.7	1178	0.0	1185	6.1	1183	39.2
75	1171	0.0	1179	0.0	1186	0.0	1190	0.0
76	1174	0.0	1188	7.5	1192	0.0	1192	0.0
77	1179	29.1	1188	0.0	1195	4.9	1203	7.0
78	1185	0.0	1192	0.0	1197	0.0	1205	0.0
79	1192	0.0	1199	0.0	1201	0.0	1208	0.0
80	1227	0.1	1240	10.5	1233	64.6	1235	376.3
81	1250	45.7	1262	0.9	1251	99.9	1241	167.2
82	1266	0.0	1273	0.0	1274	0.0	1272	0.0
83	1277	0.0	1282	0.0	1286	0.0	1279	0.0
84	1277	287.3	1287	9.0	1304	28.9	1312	3.3
85	1310	14.8	1306	1.3	1316	2.4	1316	0.7
86	1318	0.0	1330	0.0	1332	0.0	1338	0.0
87	1325	0.0	1331	1.1	1337	197.8	1342	311.6
88	1326	76.3	1345	0.0	1341	0.0	1352	0.0
89	1338	0.0	1365	0.0	1359	0.0	1354	0.0
90	1351	10.5	1374	4.2	1365	2.1	1369	373.6
91	1355	0.0	1380	0.0	1372	4.3	1375	31.3
92	1374	6.7	1390	0.0	1392	1.4	1389	0.0
93	1379	2.6	1394	2.7	1397	0.0	1397	71.2
94	1385	0.0	1397	11.4	1400	23.4	1403	57.8
95	1388	0.0	1407	0.0	1410	0.0	1406	0.0
96	1399	0.0	1412	0.0	1413	0.0	1414	0.0
97	1411	0.0	1431	4.1	1430	0.0	1430	0.0
98	1432	18.5	1432	0.0	1439	13.1	1446	6.3
99	1432	1.1	1459	0.3	1444	1.5	1446	30.4
100	1456	15.2	1479	2.8	1470	0.0	1461	0.0
101	1459	0.0	1481	0.0	1471	0.0	1471	0.0
102	1470	0.0	1487	10.5	1474	67.8	1481	97.6
103	1497	19.7	1490	0.0	1510	10.6	1512	0.0
104	1514	0.0	1542	0.0	1521	0.0	1520	55.0
105	1530	0.0	1553	7.3	1528	64.3	1523	0.0
106	1532	4.1	1557	30.6	1536	0.0	1531	0.8

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Table 1 - continued from previous page

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	1532	69.2	1557	0.0	1537	4.9	1532	0.0
108	1564	0.0	1580	0.0	1570	0.0	1565	0.0
109	1566	0.0	1586	0.0	1571	0.0	1569	457.6
110	1568	39.9	1606	5.7	1573	3.9	1571	0.0
111	1585	69.8	1606	4.1	1577	227.7	1576	500.9
112	1602	0.0	1614	0.0	1605	0.0	1606	0.0
113	3012	95.6	3042	0.7	3063	0.0	3072	0.0
114	3012	0.0	3042	0.0	3063	0.1	3072	0.1
115	3014	0.0	3044	0.0	3064	9.8	3072	0.9
116	3014	8.4	3044	38.3	3064	0.0	3072	0.0
117	3019	40.5	3045	14.3	3067	0.0	3078	0.1
118	3020	0.0	3046	0.0	3067	0.2	3078	0.0
119	3021	0.0	3048	0.0	3071	0.5	3079	0.0
120	3021	29.0	3048	0.1	3071	0.0	3079	1.3
121	3035	70.7	3057	42.5	3075	8.4	3080	0.9
122	3035	0.0	3057	0.0	3075	0.0	3080	0.0
123	3040	275.0	3064	108.6	3084	30.9	3094	0.6
124	3040	0.0	3065	0.0	3084	0.0	3094	0.0
125	3048	384.0	3075	163.0	3098	30.6	3109	1.4
126	3049	0.0	3075	0.0	3098	0.0	3109	0.0