

Harmonic vibrational frequencies of dibenzo[bc,ef]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	47	0.0	44	0.0	50	0.0	52	0.0
2	72	0.2	71	0.4	72	0.8	69	1.4
3	104	0.8	103	3.0	101	6.7	98	12.0
4	119	0.0	115	0.0	121	0.0	123	0.0
5	140	0.3	142	0.5	140	0.4	137	0.4
6	197	0.0	194	0.0	192	0.3	189	0.6
7	212	0.0	217	0.0	219	0.0	218	0.0
8	262	0.1	264	0.0	261	0.0	254	0.0
9	263	0.0	266	0.0	262	0.3	257	1.3
10	292	13.4	294	4.6	293	2.1	292	1.8
11	300	1.6	298	0.3	297	1.5	292	0.0
12	309	0.1	310	0.0	310	0.5	311	4.4
13	319	0.0	323	0.0	324	0.0	320	0.0
14	329	2.8	331	1.9	329	0.0	327	0.0
15	335	0.0	332	0.0	331	1.5	328	0.7
16	337	0.0	339	0.1	339	0.0	339	0.0
17	400	0.3	407	0.0	408	0.4	407	1.8
18	408	0.2	412	0.6	409	1.3	408	0.4
19	424	3.5	424	1.4	425	3.0	424	4.1
20	446	0.0	446	2.4	444	1.0	440	0.5
21	481	0.0	475	0.0	468	0.0	456	0.0
22	484	1.8	488	0.1	488	0.6	487	4.2
23	505	0.0	508	0.0	498	0.0	488	0.0
24	515	0.1	519	0.3	507	1.1	493	1.9
25	518	0.1	519	0.1	518	0.2	514	0.0
26	530	0.4	531	0.0	528	0.0	520	0.4
27	534	0.4	533	1.0	529	0.0	526	0.0
28	541	6.2	541	0.3	534	18.2	526	26.3
29	542	2.3	542	11.4	540	0.2	539	0.7
30	580	0.0	582	0.0	584	0.0	585	0.0
31	605	5.6	615	0.1	612	3.1	608	2.0
32	611	3.9	616	5.0	613	4.6	609	18.1
33	619	0.0	624	1.2	622	0.0	616	0.0
34	621	0.8	627	0.0	623	0.5	621	0.0
35	634	0.1	634	0.1	634	0.6	632	1.5
36	639	0.0	645	0.0	639	0.0	635	0.0
37	663	0.0	662	0.6	662	1.1	660	2.2
38	675	0.0	688	0.0	689	0.0	690	0.0
39	694	10.6	697	2.4	697	3.7	695	23.1
40	706	1.1	705	1.0	706	0.3	706	0.0
41	721	34.6	735	13.2	726	18.1	715	20.0
42	728	0.0	751	0.0	752	0.0	749	14.9
43	735	22.3	759	40.6	755	18.7	753	0.0
44	757	4.3	764	0.8	761	1.7	757	1.0
45	758	2.2	772	1.2	774	0.9	773	10.5
46	761	0.0	775	6.8	781	0.0	774	0.0
47	766	10.3	788	0.0	783	37.3	795	45.3
48	766	2.1	789	18.0	796	14.3	804	13.7
49	786	0.0	801	0.0	812	0.0	816	6.9
50	799	0.0	818	0.0	821	2.7	824	0.0
51	801	4.0	822	0.8	829	0.0	844	0.0
52	809	0.0	847	21.6	861	36.3	876	59.6

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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	816	9.3	876	0.0	889	0.0	889	1.8
54	823	51.6	880	87.4	899	0.7	897	7.9
55	841	0.0	886	1.1	899	0.0	924	0.0
56	844	93.1	899	0.1	902	71.2	930	0.0
57	885	0.4	901	0.0	924	2.2	933	39.2
58	895	0.0	905	27.5	929	0.0	954	2.7
59	918	4.1	922	7.5	934	23.5	964	0.0
60	918	0.0	952	0.0	956	0.2	967	27.8
61	928	0.0	954	1.0	977	0.0	995	0.0
62	931	0.0	973	0.0	988	0.0	1003	1.3
63	936	1.4	973	0.0	997	0.0	1003	0.0
64	936	0.0	977	2.0	999	0.0	1015	0.0
65	946	15.7	978	0.0	1001	0.5	1020	0.0
66	995	0.9	999	0.2	1004	0.5	1022	0.0
67	1035	0.7	1038	0.3	1047	0.2	1052	0.9
68	1066	1.7	1069	0.0	1074	0.3	1074	0.1
69	1082	15.9	1085	4.7	1088	2.1	1085	13.8
70	1111	0.4	1114	3.6	1123	1.4	1117	7.9
71	1113	0.0	1125	0.0	1125	1.2	1129	0.1
72	1137	0.5	1144	1.1	1152	0.0	1158	0.3
73	1155	22.9	1160	0.1	1168	2.8	1168	11.2
74	1157	0.1	1167	7.6	1169	0.0	1170	20.7
75	1179	1.4	1180	2.3	1194	1.6	1198	17.0
76	1182	6.0	1192	0.4	1195	62.4	1205	116.8
77	1194	5.0	1199	0.6	1210	2.2	1217	41.4
78	1206	5.3	1210	0.1	1216	3.4	1218	2.2
79	1214	1.6	1211	1.3	1220	4.0	1227	40.9
80	1226	1.6	1233	0.3	1234	3.3	1233	0.0
81	1235	41.2	1252	0.7	1244	130.4	1245	191.4
82	1253	53.8	1271	7.0	1267	88.5	1261	189.0
83	1262	27.2	1272	7.4	1272	0.3	1279	1.5
84	1284	7.4	1285	2.7	1293	21.0	1289	21.3
85	1293	218.5	1300	12.3	1304	111.0	1319	108.1
86	1316	78.2	1328	2.1	1332	0.0	1333	168.9
87	1318	8.7	1339	1.1	1338	39.2	1339	4.2
88	1328	77.9	1339	1.4	1348	48.5	1356	95.4
89	1333	7.7	1349	3.4	1348	16.2	1361	155.9
90	1344	32.1	1351	0.0	1359	8.2	1370	68.1
91	1356	24.3	1370	0.0	1374	24.0	1374	76.0
92	1357	5.4	1371	0.0	1380	0.1	1377	8.8
93	1371	11.0	1382	3.3	1389	5.2	1399	0.4
94	1387	29.0	1407	5.3	1402	9.6	1416	60.7
95	1392	6.5	1409	4.7	1416	9.4	1421	34.1
96	1417	0.0	1423	0.5	1429	1.5	1430	18.9
97	1424	17.0	1432	2.4	1438	0.1	1441	211.6
98	1430	1.7	1445	5.8	1445	59.3	1443	0.0
99	1441	0.3	1447	0.8	1449	11.7	1452	55.0
100	1452	0.0	1471	1.8	1462	9.2	1455	46.1
101	1452	1.9	1482	0.3	1475	1.4	1479	79.6
102	1485	4.4	1492	0.8	1489	4.6	1490	11.2
103	1495	1.8	1500	6.2	1498	0.1	1492	28.6
104	1497	1.2	1522	1.6	1509	21.3	1504	7.7
105	1536	3.5	1556	0.0	1542	51.0	1530	51.8
106	1541	5.5	1561	0.5	1542	27.4	1531	107.4

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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	1544	53.3	1570	1.1	1550	4.7	1538	17.5
108	1550	0.0	1576	4.2	1553	28.2	1546	188.5
109	1552	242.0	1591	13.9	1565	44.3	1564	182.5
110	1568	19.8	1599	3.4	1578	3.9	1568	284.8
111	1580	2.0	1605	3.5	1581	90.4	1578	8.2
112	1587	6.7	1615	13.4	1587	1.7	1595	3.6
113	3011	3.4	3043	0.1	3064	2.3	3067	0.0
114	3013	19.1	3043	1.8	3064	0.2	3067	0.6
115	3015	18.0	3045	23.4	3067	1.1	3080	0.3
116	3015	4.8	3046	1.0	3069	0.1	3080	0.2
117	3016	77.5	3046	1.7	3069	0.1	3081	0.5
118	3022	27.5	3050	2.2	3074	0.7	3082	0.6
119	3022	0.4	3051	4.0	3074	0.0	3082	0.0
120	3036	27.0	3063	4.3	3084	0.8	3094	0.0
121	3039	75.7	3065	41.8	3085	16.8	3095	0.2
122	3041	222.2	3066	100.5	3086	28.0	3095	0.2
123	3041	284.1	3066	92.3	3088	12.6	3096	0.3
124	3043	0.0	3069	14.4	3092	6.1	3103	0.4
125	3073	5.1	3082	11.2	3102	3.2	3110	0.1
126	3090	67.9	3096	45.5	3114	17.0	3119	0.2