

Harmonic vibrational frequencies of dibenzo[cd,lm]perylene (C₂₆H₁₄) 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	34	0.0	43	0.2	42	0.0	33	0.0
2	46	0.0	44	0.0	44	0.9	45	2.1
3	97	0.0	96	0.0	98	0.0	96	0.0
4	169	0.0	170	0.0	168	0.0	164	0.0
5	180	2.4	182	0.7	182	0.2	178	0.0
6	183	0.0	186	5.0	185	10.4	179	0.0
7	187	1.4	192	0.0	191	0.0	180	18.7
8	207	0.0	211	0.0	195	0.0	187	0.0
9	232	3.9	224	4.1	219	3.9	213	2.5
10	274	0.0	276	0.0	276	0.0	274	0.0
11	304	0.0	314	0.0	323	0.0	327	0.0
12	333	0.0	332	0.0	331	0.0	328	0.0
13	341	0.0	338	0.0	333	0.0	329	0.0
14	377	0.0	382	0.0	381	0.0	380	0.0
15	443	0.0	447	0.0	444	0.0	444	0.0
16	450	2.4	449	0.9	450	1.3	448	1.7
17	469	15.5	472	0.1	475	9.9	450	0.0
18	476	0.0	474	0.0	475	0.0	460	7.5
19	482	0.0	479	0.0	479	4.2	474	0.0
20	490	0.7	496	1.9	482	0.0	478	26.4
21	490	0.0	508	0.0	487	0.0	482	1.9
22	504	0.0	511	2.2	500	0.0	491	0.0
23	513	3.2	513	0.0	504	0.0	498	0.0
24	514	0.5	516	0.3	514	0.2	511	0.0
25	540	0.0	545	7.8	542	0.0	529	0.0
26	546	38.2	547	0.0	547	5.4	548	0.3
27	552	0.0	553	0.0	553	0.0	556	0.0
28	552	0.0	554	0.0	555	0.0	558	0.0
29	596	0.0	597	0.0	594	0.0	589	0.0
30	645	0.0	655	0.0	651	0.0	645	0.0
31	662	18.5	662	19.1	660	22.1	654	25.8
32	669	0.4	667	1.9	671	4.8	671	25.9
33	674	0.0	686	1.6	683	0.2	677	0.0
34	685	0.1	697	0.0	690	0.0	683	0.0
35	690	0.0	697	0.0	692	0.0	685	0.0
36	695	0.0	700	0.0	700	0.0	698	0.0
37	721	11.3	753	5.8	757	0.0	760	37.0
38	722	0.0	755	0.0	760	26.0	765	0.0
39	765	0.0	786	54.5	785	20.1	789	6.9
40	770	0.0	787	23.1	789	1.7	795	2.3
41	778	89.4	799	0.0	816	0.0	816	0.0
42	784	3.3	807	0.0	819	0.0	817	0.0
43	807	0.0	820	0.0	820	0.0	835	16.3
44	815	0.0	823	0.0	830	0.0	838	0.0
45	817	0.0	832	3.8	834	3.9	840	0.0
46	819	101.1	834	0.0	840	0.0	852	0.0
47	821	0.0	837	0.0	848	0.0	863	169.0
48	823	0.0	838	140.9	849	162.1	864	0.0
49	829	13.8	897	0.0	901	0.0	896	0.0
50	835	0.0	899	0.0	926	0.0	946	13.3
51	891	0.0	903	0.0	929	0.0	959	0.0
52	898	0.0	925	1.0	940	4.6	964	0.0

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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	905	0.0	955	0.0	971	0.0	986	0.0
54	917	0.0	956	0.0	976	0.0	996	0.5
55	920	0.2	966	0.0	982	0.2	999	0.0
56	932	0.2	970	0.0	987	0.0	1006	0.0
57	935	0.0	979	0.0	1004	0.0	1028	0.0
58	936	0.7	980	3.0	1004	0.6	1029	0.0
59	1039	47.9	1044	0.0	1047	19.4	1046	80.5
60	1043	0.0	1049	5.4	1052	0.0	1053	0.0
61	1069	0.0	1075	0.0	1078	0.0	1080	0.0
62	1103	8.7	1105	0.1	1116	40.0	1120	108.0
63	1113	7.3	1112	0.7	1123	5.8	1136	7.3
64	1136	0.0	1128	0.0	1147	0.0	1151	0.0
65	1145	0.0	1152	0.0	1160	0.0	1157	31.3
66	1149	6.7	1162	1.8	1163	1.2	1159	0.0
67	1169	0.0	1177	0.1	1177	0.0	1181	0.0
68	1173	4.2	1177	0.0	1190	0.9	1194	4.7
69	1181	0.0	1190	10.1	1202	0.0	1209	10.3
70	1197	0.2	1194	0.0	1209	42.0	1210	0.0
71	1208	1.4	1224	4.1	1225	0.1	1229	0.0
72	1219	0.0	1235	0.0	1232	0.0	1230	27.3
73	1239	0.0	1245	0.0	1248	246.2	1249	0.0
74	1240	122.9	1253	4.7	1251	0.0	1255	534.4
75	1279	0.0	1272	0.0	1289	0.0	1278	43.7
76	1281	42.6	1300	12.3	1295	10.3	1292	0.0
77	1289	0.0	1305	0.0	1303	0.0	1307	0.0
78	1310	161.4	1331	4.3	1335	56.6	1330	209.3
79	1313	0.0	1343	6.1	1339	0.0	1346	0.0
80	1315	191.8	1344	0.0	1340	70.4	1347	353.8
81	1348	4.9	1362	2.0	1367	28.5	1374	5.3
82	1349	17.6	1364	0.0	1370	0.5	1376	0.0
83	1355	0.0	1395	0.0	1386	0.0	1386	0.0
84	1362	0.0	1416	0.0	1398	0.0	1386	40.3
85	1400	1.4	1416	15.7	1419	4.1	1420	0.8
86	1417	0.0	1420	0.0	1429	0.0	1435	0.0
87	1426	0.0	1434	5.4	1441	5.1	1436	0.0
88	1429	5.0	1445	0.0	1442	0.0	1441	12.0
89	1460	0.3	1468	0.0	1467	6.7	1465	0.0
90	1471	0.0	1483	0.0	1472	0.0	1474	10.1
91	1485	0.4	1487	1.2	1493	0.6	1500	0.0
92	1487	0.0	1504	0.0	1498	0.0	1505	14.2
93	1512	2.9	1522	0.1	1520	10.1	1518	89.6
94	1529	0.0	1562	0.0	1549	0.0	1534	0.0
95	1541	205.1	1567	24.1	1549	7.7	1547	0.0
96	1548	0.0	1576	0.0	1554	0.0	1548	44.0
97	1560	30.9	1590	9.6	1556	0.0	1558	0.0
98	1562	0.0	1597	0.0	1558	162.2	1561	284.6
99	1572	277.3	1599	0.0	1573	390.5	1573	1161.3
100	1578	0.0	1619	0.1	1586	0.0	1588	0.0
101	3011	79.3	3046	2.3	3071	0.0	3079	0.1
102	3011	0.0	3047	0.0	3071	0.0	3079	0.0
103	3021	0.0	3049	0.0	3072	0.0	3081	0.0
104	3021	28.3	3050	4.3	3073	2.0	3081	0.2
105	3022	35.6	3050	14.8	3073	1.3	3082	0.0
106	3024	0.0	3052	0.0	3074	0.0	3083	0.0

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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	3031	0.0	3055	0.0	3076	0.0	3083	0.0
108	3032	150.2	3056	73.0	3076	14.5	3083	2.7
109	3046	347.3	3075	139.5	3099	33.3	3110	1.5
110	3047	0.0	3075	0.0	3099	0.0	3111	0.0
111	3060	0.0	3086	0.0	3107	0.0	3113	0.4
112	3060	14.1	3086	6.5	3107	1.8	3113	0.0
113	3078	159.8	3106	77.3	3125	19.8	3132	0.2
114	3078	0.0	3107	0.0	3125	0.0	3132	0.0