

Harmonic vibrational frequencies of dibenzo[b,def]chrysene (C₂₄H₁₄) 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	37	0.1	37	0.2	38	0.4	36	0.9
2	70	0.0	72	0.0	70	0.2	65	0.6
3	85	0.0	96	0.0	92	0.0	84	0.0
4	117	0.0	116	0.0	115	0.0	114	0.0
5	160	1.8	162	1.0	162	5.6	158	8.0
6	162	2.3	163	3.3	162	0.7	160	0.2
7	226	0.1	226	0.8	225	1.0	214	1.1
8	249	0.1	239	0.4	231	2.7	229	7.3
9	255	0.0	257	0.0	256	0.0	253	0.0
10	281	0.0	283	0.0	278	0.0	270	0.0
11	295	0.0	297	0.0	295	0.0	294	0.0
12	327	0.0	332	0.0	339	0.0	340	0.0
13	362	0.4	380	0.3	378	0.0	376	0.0
14	401	0.2	405	0.5	400	1.3	395	1.9
15	415	0.0	419	0.0	413	0.0	408	0.0
16	446	0.0	447	0.0	438	0.0	420	0.0
17	466	38.4	472	3.7	467	12.6	456	17.3
18	470	5.9	475	9.2	469	0.4	458	0.0
19	499	0.0	508	0.0	486	0.0	465	13.5
20	513	0.0	512	0.0	503	0.7	482	0.0
21	514	1.2	517	0.9	513	6.3	509	0.0
22	519	0.0	517	5.8	515	0.0	511	2.8
23	528	0.5	538	0.0	519	0.0	516	0.0
24	547	0.0	546	0.0	547	0.0	545	0.0
25	559	0.0	555	0.0	552	0.0	547	0.0
26	574	0.5	573	0.9	572	16.7	568	49.3
27	636	0.0	638	0.0	639	0.0	637	0.0
28	641	2.3	643	13.8	641	1.3	637	6.0
29	646	0.3	648	0.0	649	0.0	647	0.0
30	646	0.0	656	0.0	660	6.2	653	16.8
31	671	4.3	677	10.3	667	4.6	660	0.1
32	709	0.0	736	0.0	732	0.0	720	0.0
33	713	55.0	740	0.0	740	0.0	738	0.0
34	728	0.0	741	71.4	747	2.2	741	11.9
35	735	0.0	748	0.0	754	0.0	756	3.8
36	737	20.2	754	2.6	757	1.5	766	0.0
37	750	24.1	755	51.6	760	131.5	771	120.0
38	759	0.0	795	0.0	796	0.0	793	0.0
39	762	37.6	806	9.4	805	5.6	803	32.5
40	793	0.0	808	0.9	826	0.0	843	0.0
41	801	0.4	814	0.0	826	11.6	847	31.3
42	802	0.0	849	13.8	852	0.0	849	0.0
43	806	59.3	849	0.0	869	0.0	877	6.5
44	838	35.5	849	0.0	870	11.7	890	6.3
45	839	0.0	879	3.4	879	1.7	890	0.0
46	846	0.0	890	61.4	914	45.5	952	24.5
47	874	0.6	893	0.0	915	0.0	953	0.0
48	889	9.2	946	0.0	965	0.0	964	0.0
49	890	0.0	948	6.7	966	0.0	984	0.0
50	909	0.5	963	0.0	969	7.1	991	7.4
51	915	0.0	964	0.1	981	0.3	992	13.5
52	937	0.0	969	0.0	985	0.0	1000	5.6

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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	938	0.3	982	0.4	992	4.4	1004	0.0
54	959	0.0	987	0.0	1012	0.0	1027	70.8
55	981	19.1	987	0.3	1012	0.0	1032	0.0
56	1025	29.6	1022	7.5	1030	1.8	1032	0.3
57	1029	0.0	1023	0.0	1033	0.0	1034	0.0
58	1047	0.6	1047	0.3	1056	1.0	1057	5.8
59	1085	0.0	1088	0.0	1098	0.0	1094	0.0
60	1122	1.8	1121	0.0	1137	0.7	1130	8.3
61	1131	0.0	1139	0.9	1141	0.0	1150	0.0
62	1145	0.0	1161	0.0	1159	0.0	1158	0.0
63	1167	0.0	1169	2.7	1187	0.4	1193	0.0
64	1167	9.8	1180	0.0	1188	0.0	1194	69.6
65	1184	151.4	1185	2.4	1195	189.8	1202	26.7
66	1187	6.8	1206	12.6	1207	11.4	1211	0.0
67	1198	0.0	1213	0.0	1213	0.0	1213	326.8
68	1248	16.5	1239	1.8	1260	24.4	1256	0.0
69	1252	0.0	1249	0.0	1264	0.0	1272	100.2
70	1255	0.0	1272	0.0	1270	0.0	1282	0.0
71	1271	14.5	1282	7.7	1286	0.5	1288	48.3
72	1278	56.9	1304	5.6	1293	20.5	1291	10.8
73	1300	0.0	1322	0.0	1313	0.0	1302	0.0
74	1313	242.2	1327	0.0	1333	0.0	1331	488.0
75	1318	594.0	1349	0.0	1334	551.9	1341	0.0
76	1318	0.0	1354	6.5	1351	0.0	1357	403.6
77	1330	0.0	1365	0.0	1351	49.6	1361	0.0
78	1350	0.0	1365	0.9	1369	0.0	1373	0.0
79	1391	0.0	1416	0.0	1415	0.0	1419	0.0
80	1397	38.3	1418	1.4	1423	2.5	1420	22.8
81	1413	58.7	1423	0.2	1427	59.8	1434	29.0
82	1424	0.0	1428	0.0	1436	0.0	1442	0.0
83	1437	131.2	1455	11.0	1446	7.7	1458	14.0
84	1461	0.0	1470	0.0	1468	0.0	1462	0.0
85	1472	17.1	1473	3.4	1480	183.7	1487	804.0
86	1484	0.0	1497	0.0	1499	0.0	1495	0.0
87	1510	5.3	1515	6.2	1520	23.7	1514	0.0
88	1514	0.0	1542	0.0	1534	0.0	1515	65.4
89	1531	339.6	1568	0.0	1535	203.4	1529	64.9
90	1532	0.0	1577	2.9	1542	0.0	1536	0.0
91	1540	64.1	1584	2.3	1543	161.3	1545	856.5
92	1550	0.0	1601	0.0	1564	0.0	1559	0.0
93	1566	56.1	1610	13.9	1579	99.3	1565	255.8
94	1584	0.0	1616	0.0	1590	0.0	1589	0.0
95	3012	12.4	3043	4.5	3062	1.3	3065	0.8
96	3012	0.0	3043	0.0	3062	0.0	3065	0.0
97	3016	0.0	3047	0.0	3071	0.0	3082	0.0
98	3016	7.9	3047	7.9	3071	4.6	3082	0.6
99	3021	80.2	3050	27.8	3073	4.3	3082	1.0
100	3022	0.0	3051	0.0	3074	0.0	3082	0.0
101	3028	0.0	3057	0.0	3081	0.0	3091	0.0
102	3029	143.7	3057	44.8	3081	4.7	3091	2.3
103	3043	256.5	3074	87.0	3096	13.9	3105	0.1
104	3044	0.0	3074	0.0	3096	0.0	3105	0.0
105	3056	63.1	3084	36.7	3103	24.3	3112	0.0
106	3056	0.0	3084	0.0	3103	0.0	3112	1.0

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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})
107	3071	204.2	3099	86.2	3117	22.9	3121	0.6
108	3072	0.0	3100	0.0	3117	0.0	3122	0.0