

Harmonic vibrational frequencies of chrysene (C₁₈H₁₂) 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	28	0.1	49	0.1	40	0.1	19	0.0
2	74	0.1	76	0.2	74	0.8	70	1.8
3	117	0.0	133	0.0	128	0.0	113	0.0
4	182	0.0	174	0.0	167	0.0	163	0.0
5	183	3.3	185	0.5	183	0.1	179	0.1
6	226	1.6	233	4.4	219	7.9	203	11.0
7	284	0.0	289	0.0	282	0.0	278	0.0
8	285	0.1	289	0.1	288	1.7	280	6.5
9	352	0.0	378	0.0	370	0.0	351	0.0
10	369	0.0	384	0.0	372	0.0	365	0.0
11	414	5.3	431	8.0	414	6.8	392	6.1
12	473	4.8	476	0.0	451	0.0	419	0.0
13	474	0.0	480	8.4	472	0.0	424	3.9
14	480	0.0	481	0.0	474	11.5	463	0.0
15	511	0.0	510	0.0	492	0.0	466	0.0
16	528	1.1	538	2.1	512	8.4	470	19.1
17	537	21.0	554	2.3	536	7.8	522	8.0
18	561	0.9	571	0.8	543	0.8	535	4.6
19	562	46.8	571	0.0	553	0.0	548	0.0
20	564	0.0	579	4.9	565	19.9	557	55.8
21	650	0.0	675	0.0	675	0.0	659	0.0
22	670	0.0	679	0.0	675	0.0	667	0.0
23	671	59.2	685	11.0	679	6.2	673	4.9
24	695	0.1	732	0.0	727	10.6	711	32.7
25	701	0.0	740	0.0	752	0.0	752	0.0
26	729	128.5	762	97.5	760	95.4	761	0.0
27	734	0.0	770	0.0	768	0.0	769	81.1
28	752	32.9	777	0.0	771	0.0	772	0.0
29	755	0.0	816	64.3	836	64.2	843	76.1
30	764	0.0	826	0.0	840	0.0	855	61.5
31	823	11.0	850	2.2	849	12.8	856	0.0
32	826	0.0	863	9.2	867	0.0	869	0.0
33	836	2.0	868	0.0	877	14.8	871	37.0
34	856	3.9	874	0.0	883	10.5	903	0.0
35	858	0.0	877	3.6	886	0.0	904	12.2
36	859	0.0	939	0.0	960	0.0	979	0.0
37	871	15.7	946	4.1	967	3.4	986	3.1
38	874	10.5	958	0.3	980	0.2	998	0.0
39	879	0.0	968	0.0	987	0.0	1007	0.8
40	918	0.0	987	0.0	1011	0.0	1011	0.0
41	919	0.0	988	0.2	1014	0.0	1032	95.2
42	996	0.0	1016	0.0	1014	0.0	1033	0.0
43	1035	76.2	1032	6.9	1039	28.3	1034	0.8
44	1040	0.0	1040	0.0	1047	0.0	1039	0.0
45	1073	12.2	1078	0.4	1086	14.1	1076	63.8
46	1108	0.0	1141	0.0	1131	0.0	1116	0.0
47	1118	0.0	1158	0.5	1146	73.8	1125	125.8
48	1127	35.1	1171	2.8	1153	0.0	1125	0.0
49	1161	0.0	1179	0.0	1188	12.2	1193	0.0
50	1163	12.9	1186	0.0	1191	0.0	1198	56.8
51	1200	0.0	1196	2.3	1225	367.7	1211	249.2
52	1206	449.1	1230	0.0	1235	0.0	1240	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})
53	1237	8.0	1240	3.0	1254	22.1	1263	51.7
54	1238	0.0	1260	0.0	1266	28.5	1278	0.0
55	1250	143.8	1263	15.8	1267	0.0	1291	0.0
56	1278	0.0	1303	0.0	1302	18.2	1298	47.2
57	1279	389.9	1322	0.0	1315	0.0	1301	84.5
58	1296	536.6	1347	2.7	1331	488.2	1349	0.0
59	1316	0.0	1356	0.0	1343	0.0	1361	332.2
60	1329	0.0	1362	0.0	1359	0.0	1376	0.0
61	1410	161.3	1426	10.3	1425	0.0	1394	0.0
62	1411	0.0	1434	4.7	1427	74.9	1434	0.0
63	1420	0.0	1437	0.0	1436	0.0	1435	24.4
64	1430	126.9	1457	0.0	1444	47.4	1456	50.0
65	1454	0.0	1485	8.6	1486	0.0	1485	621.7
66	1478	3.7	1514	9.4	1493	161.2	1490	0.0
67	1490	143.9	1519	0.0	1507	217.6	1517	0.0
68	1508	0.0	1552	0.0	1530	0.0	1522	439.1
69	1520	506.9	1589	8.1	1536	418.2	1536	106.9
70	1530	0.0	1598	0.0	1549	0.0	1546	0.0
71	1541	31.3	1606	2.0	1559	130.3	1551	376.6
72	1567	0.0	1608	0.0	1576	0.0	1582	0.0
73	3003	0.0	3045	0.0	3073	0.0	3077	3.8
74	3004	25.4	3045	1.0	3073	0.4	3077	0.1
75	3013	27.8	3049	20.7	3075	5.9	3084	3.8
76	3014	0.0	3050	0.0	3076	0.0	3084	0.0
77	3019	0.0	3056	0.0	3084	0.0	3093	0.0
78	3020	144.6	3057	43.9	3084	1.5	3093	6.9
79	3036	256.7	3074	81.5	3097	3.3	3104	0.0
80	3038	0.0	3074	0.0	3098	0.0	3104	0.1
81	3045	0.0	3084	0.0	3105	0.0	3114	0.5
82	3046	111.6	3084	19.7	3105	25.6	3114	10.6
83	3065	159.5	3100	68.9	3118	0.0	3120	0.0
84	3066	0.0	3101	0.0	3118	12.0	3120	1.9