

Harmonic vibrational frequencies of perylene (C₂₀H₁₂) 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	31	0.0	25	0.0	46	0.0	52	0.0
2	92	0.0	94	0.6	89	1.5	84	3.2
3	136	0.0	127	0.0	140	0.0	143	0.0
4	182	2.5	174	4.8	169	8.3	161	12.2
5	194	0.0	204	0.0	199	0.0	193	0.0
6	216	0.0	235	0.0	240	0.0	243	0.0
7	252	1.9	250	0.2	249	1.1	245	1.2
8	289	0.0	291	0.0	275	0.0	258	0.0
9	348	0.0	348	0.0	351	0.0	349	0.0
10	359	0.0	359	0.0	363	0.0	366	0.0
11	388	0.0	417	0.0	406	0.0	393	0.0
12	431	0.0	429	0.0	429	0.0	427	0.0
13	457	22.2	454	0.0	448	0.0	433	11.3
14	489	3.0	462	2.5	458	1.9	435	0.0
15	490	0.0	472	0.3	459	0.4	455	0.7
16	503	0.0	528	0.0	505	0.0	475	0.0
17	531	0.9	536	0.9	525	1.5	507	7.3
18	537	0.0	540	0.0	526	9.3	513	4.0
19	540	1.4	540	0.0	535	0.0	528	0.0
20	541	0.0	544	8.2	540	0.0	538	0.0
21	566	0.5	579	3.0	576	6.9	568	16.4
22	611	0.0	630	0.0	614	0.0	593	0.0
23	620	0.0	634	0.0	629	0.0	624	0.0
24	629	0.0	639	0.0	636	0.0	624	0.0
25	636	0.0	648	0.0	642	0.0	645	0.0
26	704	0.0	751	0.0	742	73.4	720	77.9
27	710	0.0	752	0.0	743	0.0	738	0.0
28	729	0.0	765	64.7	765	6.0	752	27.1
29	737	135.8	771	0.0	767	0.0	782	0.0
30	765	2.6	774	2.7	792	0.0	791	7.3
31	779	39.9	792	7.9	793	0.7	797	0.0
32	780	0.0	798	0.0	799	0.0	798	39.6
33	789	2.2	806	4.0	805	4.0	811	0.0
34	791	0.0	814	118.1	813	114.2	814	111.1
35	794	13.8	843	0.0	844	0.0	848	0.0
36	794	0.0	881	0.0	911	0.0	943	0.0
37	807	0.0	890	0.0	918	0.0	945	0.0
38	825	15.7	901	0.0	935	0.0	950	0.0
39	826	0.0	909	0.4	941	3.3	971	0.0
40	912	0.0	953	0.0	951	0.0	976	4.9
41	917	0.0	968	0.0	981	0.0	985	0.0
42	919	0.0	969	0.0	997	0.0	1012	57.7
43	925	1.5	973	0.0	1002	0.0	1022	0.0
44	943	0.0	978	0.0	1007	0.0	1027	0.0
45	966	0.0	981	2.5	1009	0.1	1032	0.0
46	1017	67.1	1042	3.2	1030	20.9	1033	0.5
47	1055	0.0	1052	0.0	1063	0.0	1058	0.0
48	1088	6.7	1091	2.5	1100	0.8	1098	9.4
49	1097	0.0	1100	0.0	1108	0.0	1106	0.0
50	1114	0.1	1134	4.1	1130	17.1	1115	30.1
51	1134	0.0	1156	1.1	1150	0.0	1132	0.0
52	1145	16.6	1157	0.0	1162	2.9	1167	2.7

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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	1180	0.0	1199	0.0	1199	0.0	1201	0.0
54	1189	0.0	1199	0.0	1207	58.5	1214	101.3
55	1192	7.1	1200	1.2	1214	0.0	1223	0.0
56	1205	0.0	1216	5.8	1227	1.4	1234	34.3
57	1208	0.0	1217	0.1	1231	8.3	1234	2.5
58	1224	0.0	1229	0.0	1238	0.0	1246	0.0
59	1268	148.8	1270	2.8	1291	149.7	1283	0.0
60	1283	0.0	1303	0.0	1298	0.0	1316	211.7
61	1299	203.9	1329	8.6	1331	173.4	1328	492.1
62	1319	10.7	1342	0.0	1338	0.1	1362	28.5
63	1339	0.0	1349	2.8	1364	0.0	1377	0.0
64	1342	0.0	1354	0.0	1365	0.0	1386	0.0
65	1352	0.0	1358	0.0	1373	0.0	1391	7.7
66	1369	6.2	1386	36.2	1390	41.2	1408	0.0
67	1405	1.0	1443	0.0	1442	1.3	1425	77.3
68	1431	2.9	1446	3.7	1446	8.7	1438	0.0
69	1437	0.0	1456	0.0	1449	0.0	1444	0.0
70	1446	0.0	1468	1.6	1459	0.0	1476	0.0
71	1482	0.5	1495	6.2	1487	1.4	1480	29.9
72	1518	0.0	1514	0.0	1521	0.0	1503	235.4
73	1531	168.9	1551	0.0	1539	176.0	1514	0.0
74	1534	12.7	1572	9.8	1544	103.8	1517	0.0
75	1537	0.0	1586	23.7	1546	0.0	1548	0.0
76	1538	0.0	1586	0.0	1553	0.0	1555	448.1
77	1554	167.3	1596	9.5	1560	7.9	1560	38.6
78	1556	0.0	1607	0.0	1565	0.0	1585	0.0
79	3004	0.0	3048	0.0	3076	0.0	3082	0.1
80	3005	130.0	3049	7.4	3076	0.0	3082	0.0
81	3006	20.6	3050	0.1	3078	0.2	3084	9.1
82	3007	0.0	3051	0.0	3079	0.0	3084	0.0
83	3029	0.0	3065	0.0	3093	0.0	3102	10.3
84	3030	69.6	3067	130.5	3093	13.4	3102	0.0
85	3034	345.4	3068	34.2	3096	4.1	3106	8.7
86	3036	0.0	3071	0.0	3097	0.0	3106	0.0
87	3066	0.0	3083	0.0	3109	0.0	3115	1.6
88	3067	12.4	3084	12.7	3109	2.5	3115	0.0
89	3084	136.8	3098	69.6	3123	14.0	3130	1.8
90	3085	0.0	3099	0.0	3124	0.0	3131	0.0