

Harmonic vibrational frequencies of pyrene (C₁₆H₁₀) 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	103	0.1	98	0.4	100	1.5	100	3.2
2	144	0.0	151	0.0	145	0.0	138	0.0
3	214	2.7	209	7.3	197	13.4	186	21.4
4	216	0.0	246	0.0	241	0.0	232	0.0
5	264	0.0	259	0.0	251	0.0	238	0.0
6	346	14.2	353	1.4	349	0.7	343	0.2
7	379	0.0	396	0.0	390	0.0	384	0.0
8	402	0.0	406	0.0	408	0.0	408	0.0
9	449	0.0	455	0.0	453	0.0	424	9.3
10	481	0.0	491	1.5	465	0.8	435	0.0
11	488	7.1	500	2.5	473	0.0	446	0.0
12	496	0.0	502	0.0	495	0.0	492	0.0
13	503	7.8	504	0.0	498	5.7	496	4.1
14	520	0.0	527	0.0	526	0.0	499	0.0
15	540	0.3	549	2.5	536	0.5	520	0.0
16	566	0.0	577	0.0	545	0.0	525	4.3
17	574	0.0	579	0.0	582	0.0	583	0.0
18	650	0.0	678	0.0	665	0.0	646	0.0
19	679	12.7	693	0.1	683	9.6	665	54.5
20	684	49.4	711	32.1	684	49.2	671	44.7
21	702	0.0	739	0.0	732	0.0	720	0.0
22	706	5.9	746	10.0	754	0.0	751	0.0
23	726	0.0	771	0.0	767	4.3	790	2.8
24	729	0.0	803	0.0	805	0.0	802	0.0
25	749	0.0	804	0.0	817	3.4	813	24.8
26	790	0.0	820	3.1	821	0.0	825	0.0
27	799	110.1	827	0.0	827	0.0	845	0.0
28	799	0.0	848	120.2	863	116.8	880	110.0
29	809	0.8	895	0.0	929	0.0	964	48.3
30	816	0.0	909	0.0	942	0.0	970	0.0
31	877	0.0	955	0.2	966	12.0	979	102.4
32	884	0.0	966	0.0	983	0.0	987	0.0
33	918	0.0	973	0.0	985	19.5	996	0.0
34	918	0.0	976	2.6	993	0.0	1016	0.0
35	947	5.4	985	0.0	1006	0.0	1036	0.9
36	969	40.8	996	0.6	1010	0.0	1037	0.0
37	1057	0.0	1066	0.0	1068	0.0	1066	0.0
38	1082	1.5	1092	4.8	1098	9.6	1102	17.8
39	1108	0.0	1107	0.0	1127	0.0	1115	49.7
40	1129	0.0	1151	0.0	1149	0.0	1133	0.0
41	1144	8.1	1161	1.6	1155	0.4	1137	0.0
42	1160	1.5	1183	0.0	1186	0.0	1197	0.0
43	1169	0.0	1188	10.3	1196	4.3	1200	0.0
44	1198	0.3	1207	0.0	1214	17.9	1205	1.9
45	1216	0.0	1241	0.0	1232	0.0	1223	0.0
46	1223	0.0	1251	0.0	1242	0.0	1225	37.0
47	1245	17.7	1253	3.6	1250	85.4	1251	260.5
48	1287	298.9	1314	6.5	1335	0.0	1328	0.0
49	1315	0.0	1324	0.0	1336	0.0	1340	275.9
50	1319	0.0	1361	0.0	1339	140.4	1347	0.0
51	1340	0.0	1389	0.0	1384	0.0	1374	0.0
52	1371	0.8	1415	0.0	1412	20.3	1424	9.1

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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	1400	1.4	1427	11.8	1426	0.0	1430	75.4
54	1407	0.0	1427	1.2	1433	33.3	1432	0.0
55	1431	0.5	1445	0.5	1437	3.3	1439	12.6
56	1456	1.3	1476	4.0	1471	0.1	1481	11.0
57	1481	0.0	1498	0.0	1482	0.0	1482	0.0
58	1501	0.0	1551	0.0	1517	0.0	1501	0.0
59	1507	0.0	1571	0.0	1532	202.2	1518	390.4
60	1524	170.5	1586	12.8	1538	0.0	1542	0.0
61	1544	48.8	1597	5.5	1538	17.5	1544	116.7
62	1592	0.0	1618	0.0	1602	0.0	1597	0.0
63	2990	107.9	3042	3.6	3074	0.1	3079	1.3
64	2991	0.0	3042	0.0	3074	0.0	3079	0.0
65	2996	0.0	3046	0.0	3077	0.0	3080	0.0
66	2997	13.8	3046	0.0	3077	0.1	3080	12.0
67	3017	1.7	3053	25.3	3080	1.3	3084	5.0
68	3020	0.0	3054	0.0	3080	0.0	3084	0.0
69	3022	0.0	3063	92.5	3089	6.8	3094	22.0
70	3024	312.8	3064	0.0	3089	0.0	3094	0.0
71	3033	277.6	3074	95.8	3104	4.2	3112	29.1
72	3036	0.0	3074	0.0	3104	0.0	3112	0.0