

Harmonic vibrational frequencies of phenanthrene (C<sub>14</sub>H<sub>10</sub>) 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 <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )	Freq. (cm <sup>-1</sup> )	Int. (km mol <sup>-1</sup> )
1	65	0.0	95	0.0	81	0.0	58	0.0
2	105	0.6	100	0.7	100	1.4	101	2.3
3	213	0.1	226	2.9	211	7.0	191	11.5
4	243	2.4	240	0.0	232	0.0	220	0.0
5	247	0.0	243	0.4	240	0.0	233	0.1
6	360	0.0	394	0.0	376	0.0	345	0.0
7	399	0.7	404	0.4	401	0.1	377	13.3
8	418	3.2	430	5.5	407	10.0	388	0.0
9	418	12.2	440	1.7	431	0.5	394	0.0
10	493	19.0	498	3.9	471	0.2	417	3.9
11	494	0.0	500	0.8	477	0.0	424	0.1
12	500	8.5	534	0.0	490	2.3	493	0.1
13	544	0.4	550	0.3	543	0.0	497	0.0
14	568	0.0	593	0.0	547	0.8	543	1.2
15	619	0.6	627	4.6	597	46.2	587	76.5
16	663	12.4	708	0.1	693	39.0	662	48.0
17	678	0.0	715	1.3	697	0.0	683	0.0
18	689	63.0	717	2.4	710	1.5	698	4.9
19	692	69.8	736	75.2	758	0.0	731	0.0
20	694	0.0	756	0.0	758	56.9	777	0.0
21	715	22.9	788	0.0	764	0.0	783	59.9
22	744	0.0	817	59.2	831	0.1	822	0.6
23	768	0.0	830	0.1	839	53.6	844	44.2
24	791	42.4	867	0.0	859	8.4	859	45.7
25	806	0.0	870	1.5	884	0.0	905	0.0
26	822	3.7	871	11.1	890	7.1	913	8.8
27	848	0.0	939	0.0	963	0.0	976	103.8
28	857	0.6	950	4.4	976	4.1	987	0.0
29	864	5.8	972	0.0	986	31.5	1001	4.6
30	916	0.0	987	0.0	987	0.0	1012	27.7
31	917	0.1	988	0.0	1014	0.0	1017	0.0
32	967	91.4	999	1.4	1015	1.1	1019	25.8
33	1025	1.2	1036	0.6	1033	5.5	1036	0.0
34	1026	19.9	1039	3.6	1035	3.4	1038	4.4
35	1068	2.3	1093	0.8	1089	0.1	1072	3.2
36	1110	7.5	1148	1.3	1139	10.9	1084	12.0
37	1115	164.7	1163	0.2	1139	3.9	1131	62.7
38	1120	48.5	1173	0.0	1154	159.2	1171	181.1
39	1158	4.0	1182	0.7	1190	1.7	1191	2.3
40	1193	40.7	1203	2.0	1218	16.0	1206	11.7
41	1207	2.3	1225	0.9	1231	44.5	1235	74.5
42	1249	0.4	1250	9.3	1262	30.3	1265	19.7
43	1263	255.0	1288	0.1	1292	61.7	1302	37.5
44	1267	0.0	1298	1.6	1297	0.6	1303	64.7
45	1281	93.8	1335	0.1	1309	186.0	1341	246.7
46	1328	9.4	1342	2.2	1353	0.2	1375	2.8
47	1392	0.4	1417	0.9	1412	2.2	1405	139.2
48	1402	9.3	1421	0.7	1420	80.8	1417	2.5
49	1413	6.1	1444	3.6	1429	0.8	1439	12.3
50	1423	0.0	1462	14.2	1435	0.1	1449	4.5
51	1463	97.0	1497	7.1	1496	15.9	1500	171.7
52	1490	2.6	1521	1.8	1512	7.4	1502	7.9

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Table 1 - continued from previous page

Numb. of the mode	Anion		Neutral		Cation		Dication	
	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )	Freq. ( $\text{cm}^{-1}$ )	Int. ( $\text{km mol}^{-1}$ )
53	1492	189.6	1554	0.0	1513	10.1	1522	51.3
54	1523	177.3	1595	4.4	1533	113.5	1541	38.4
55	1530	17.2	1604	0.6	1550	183.5	1565	156.8
56	1575	18.1	1610	0.8	1583	23.8	1579	108.2
57	2988	95.8	3041	0.6	3074	0.6	3078	0.6
58	2990	4.8	3045	5.2	3078	0.2	3084	0.0
59	2994	4.2	3046	2.8	3079	0.9	3085	3.4
60	3013	13.3	3055	0.1	3085	0.0	3087	17.9
61	3013	12.5	3057	19.8	3087	0.2	3088	1.2
62	3021	183.2	3064	45.8	3089	1.4	3089	18.7
63	3022	209.8	3070	50.8	3098	0.1	3102	0.0
64	3031	7.8	3075	2.9	3106	0.7	3113	1.9
65	3045	83.7	3082	38.2	3109	7.4	3115	33.6
66	3055	86.5	3093	32.8	3113	3.0	3116	2.5