

Harmonic vibrational frequencies of benzo[e]pyrene (C<sub>20</sub>H<sub>12</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	50	0.0	49	0.0	57	0.0	58	0.0
2	75	0.0	77	0.0	76	0.0	68	0.0
3	128	0.7	125	2.6	122	6.4	120	11.8
4	142	0.0	159	0.0	153	0.0	144	0.0
5	199	0.3	219	1.8	214	3.0	206	4.1
6	251	1.1	251	0.3	246	4.0	240	13.9
7	274	0.8	276	0.5	261	0.6	247	0.7
8	278	0.0	287	0.0	278	0.0	262	0.0
9	333	12.2	336	0.3	336	0.3	333	0.0
10	378	7.6	380	0.8	380	0.4	379	0.0
11	398	0.5	404	0.0	396	2.1	379	19.3
12	403	0.0	423	0.0	409	0.0	395	0.0
13	423	1.8	428	0.7	422	0.0	405	3.1
14	448	1.5	450	0.5	449	1.2	442	4.3
15	485	4.3	490	0.6	469	1.0	446	4.0
16	504	7.1	507	1.1	498	0.0	458	0.0
17	512	0.0	527	0.0	502	1.9	494	0.0
18	549	1.3	557	4.8	533	0.0	500	0.3
19	551	2.3	563	0.4	549	0.9	542	5.4
20	554	6.0	567	0.0	560	0.5	554	3.4
21	560	0.0	569	6.5	566	9.3	557	10.1
22	613	0.8	621	0.0	613	1.4	606	0.0
23	621	0.0	644	0.0	627	0.0	606	0.7
24	645	1.2	651	3.4	644	14.7	632	25.4
25	671	45.2	704	6.7	679	23.3	661	29.2
26	674	0.0	713	0.0	704	16.1	693	52.1
27	701	17.4	737	0.0	741	0.0	740	0.0
28	711	37.0	751	92.5	749	0.0	745	108.9
29	727	0.0	768	0.0	758	102.2	746	0.0
30	733	44.1	772	8.4	761	21.6	763	107.2
31	750	0.7	776	1.8	776	7.2	771	21.7
32	763	0.0	780	0.1	786	0.3	802	0.3
33	764	9.8	823	0.0	818	0.0	822	0.0
34	772	1.9	832	68.5	847	61.6	859	81.5
35	799	55.8	860	0.0	866	0.0	862	56.7
36	805	0.0	870	0.2	868	23.0	867	0.0
37	824	0.0	892	0.0	922	0.0	943	47.6
38	862	7.3	899	6.5	926	6.2	962	0.0
39	880	0.0	939	0.2	945	13.8	964	6.8
40	902	1.1	947	1.0	965	0.3	982	0.2
41	919	0.0	966	0.0	985	0.0	984	103.2
42	922	0.3	973	1.8	987	31.0	1002	0.0
43	934	55.2	980	0.0	1000	0.0	1011	34.1
44	935	0.0	984	0.0	1003	0.0	1026	0.0
45	968	86.8	998	0.4	1012	0.0	1026	1.4
46	1020	38.1	1037	3.4	1029	4.3	1027	1.2
47	1040	4.6	1070	0.6	1053	1.4	1029	0.0
48	1057	42.8	1077	0.8	1074	6.1	1057	81.6
49	1078	0.2	1087	0.2	1088	2.1	1087	3.3
50	1100	0.3	1108	3.0	1113	9.2	1116	12.1
51	1140	36.1	1160	2.0	1157	6.1	1138	56.1
52	1143	17.5	1163	2.0	1163	0.3	1157	142.7

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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	1168	8.4	1184	0.0	1191	6.2	1174	88.6
54	1178	25.0	1203	4.0	1207	87.8	1196	22.2
55	1189	81.2	1207	0.9	1211	15.8	1215	20.6
56	1207	7.8	1214	0.0	1228	5.6	1225	102.2
57	1212	2.4	1248	0.2	1230	0.4	1227	11.1
58	1233	15.6	1251	0.6	1254	1.3	1262	83.7
59	1248	58.2	1275	1.7	1268	48.4	1266	26.6
60	1277	411.0	1297	0.2	1302	92.2	1300	167.6
61	1282	83.5	1314	4.1	1313	180.5	1325	344.1
62	1307	176.6	1317	4.5	1328	75.0	1335	10.4
63	1325	0.3	1324	2.5	1342	7.8	1347	64.2
64	1330	4.8	1352	0.4	1347	50.6	1359	189.2
65	1357	22.9	1394	1.5	1390	54.2	1398	6.4
66	1382	12.0	1406	14.8	1408	42.4	1408	62.0
67	1399	11.0	1431	0.9	1436	42.7	1433	67.2
68	1425	4.1	1439	9.0	1439	1.3	1442	0.5
69	1441	15.5	1465	19.0	1440	0.6	1446	27.0
70	1456	98.4	1472	0.0	1479	3.5	1478	40.4
71	1465	29.8	1499	0.2	1489	9.9	1483	57.3
72	1484	0.4	1512	4.0	1492	10.0	1484	8.1
73	1491	0.0	1556	0.0	1504	13.3	1504	23.4
74	1523	190.9	1567	2.3	1532	112.6	1515	110.4
75	1523	23.2	1581	0.7	1539	116.6	1529	277.5
76	1546	57.0	1589	13.0	1543	15.4	1539	52.6
77	1563	4.8	1598	0.1	1584	0.7	1570	24.8
78	1577	24.5	1615	1.0	1585	29.3	1579	51.6
79	2999	132.8	3043	2.2	3073	0.0	3082	0.1
80	3000	0.5	3049	4.3	3078	0.5	3083	3.7
81	3003	0.0	3049	0.9	3079	0.1	3085	2.9
82	3016	23.7	3054	1.7	3081	0.3	3094	0.0
83	3026	9.2	3064	4.8	3089	5.4	3095	7.8
84	3031	133.8	3067	92.4	3092	4.2	3101	5.6
85	3033	231.4	3067	58.6	3096	6.0	3106	5.4
86	3037	3.8	3070	0.0	3098	0.1	3107	0.0
87	3059	1.0	3084	0.8	3105	0.0	3114	7.8
88	3063	14.5	3087	4.6	3108	6.7	3115	0.0
89	3079	100.2	3101	54.2	3123	12.9	3130	0.4
90	3082	70.1	3104	22.7	3124	7.6	3131	0.1