

Harmonic vibrational frequencies of anthanthrene ($C_{22}H_{12}$) 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	68	0.0	65	0.4	66	1.5	66	3.6
2	94	0.2	96	0.5	94	0.6	92	0.6
3	164	0.0	160	0.0	159	0.0	156	0.0
4	184	2.0	183	5.5	178	10.0	172	15.9
5	190	0.0	198	0.0	195	0.0	189	0.0
6	259	8.6	262	2.1	261	1.6	259	1.2
7	270	0.0	281	0.0	277	0.0	269	0.0
8	282	0.0	286	0.1	282	0.7	274	1.0
9	316	1.6	310	0.3	310	0.2	305	2.7
10	337	0.0	339	0.0	339	0.0	338	0.0
11	379	0.0	383	0.0	381	0.0	379	0.0
12	380	0.0	390	0.0	392	0.0	394	0.0
13	446	0.0	448	0.0	446	0.0	443	0.0
14	467	4.4	467	4.3	466	4.3	450	3.1
15	468	1.3	484	2.1	467	2.9	463	0.0
16	497	1.2	498	1.7	488	0.0	463	3.3
17	500	0.0	502	0.0	496	2.2	493	4.8
18	519	0.0	518	0.0	506	0.0	502	0.0
19	519	0.0	521	0.0	522	0.0	518	3.6
20	538	3.9	543	3.9	535	0.1	522	0.0
21	548	0.0	548	0.0	549	0.0	546	12.2
22	554	18.7	555	1.5	556	8.5	547	0.0
23	565	0.6	564	1.5	557	0.5	556	8.8
24	597	0.1	602	1.7	597	3.5	590	11.8
25	623	0.0	637	0.0	629	0.0	618	0.0
26	647	0.0	652	0.0	649	0.0	645	0.0
27	675	4.6	687	10.7	679	0.0	667	0.0
28	684	0.0	690	0.0	680	18.7	675	28.6
29	715	0.0	735	1.9	740	2.9	740	25.7
30	715	54.2	753	0.0	745	35.1	741	44.1
31	734	6.3	753	0.0	752	0.0	747	0.0
32	749	0.0	754	41.7	760	3.0	756	5.3
33	754	0.9	761	1.3	766	0.0	779	0.0
34	756	10.9	790	4.0	796	0.0	805	0.0
35	769	0.0	797	0.0	799	0.5	808	1.7
36	783	1.3	808	34.8	819	0.0	817	0.0
37	786	0.0	819	0.0	823	53.3	838	67.2
38	808	4.8	828	0.0	840	0.0	854	0.0
39	811	0.0	874	0.0	897	2.1	897	16.0
40	816	0.0	887	94.7	900	0.0	934	0.0
41	828	135.8	895	1.7	909	85.2	939	64.9
42	834	0.0	901	7.9	936	2.4	958	44.4
43	888	18.9	911	0.0	944	0.0	975	1.2
44	922	0.5	951	0.7	958	8.0	986	0.0
45	922	0.0	971	0.0	989	0.0	987	0.0
46	927	0.6	972	2.0	990	0.3	1002	0.0
47	929	0.0	979	1.4	991	0.0	1007	0.9
48	948	2.1	982	0.0	1005	0.5	1032	0.0
49	979	0.0	990	0.0	1007	0.0	1032	0.0
50	1036	0.0	1043	0.0	1047	0.0	1048	0.0
51	1059	13.0	1065	1.1	1070	0.8	1072	8.3
52	1080	0.9	1077	5.1	1091	4.9	1099	8.5

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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	1084	0.0	1091	0.0	1097	0.0	1100	0.0
54	1140	7.0	1147	3.2	1154	8.8	1151	31.2
55	1151	0.0	1158	0.0	1165	0.0	1165	0.0
56	1166	0.4	1174	3.5	1188	9.8	1190	0.0
57	1170	0.0	1181	0.0	1189	0.0	1197	32.5
58	1182	0.0	1189	8.0	1199	12.6	1202	0.0
59	1183	18.8	1197	0.0	1200	0.0	1206	2.3
60	1214	0.0	1229	0.0	1225	0.0	1218	0.0
61	1230	62.6	1249	4.6	1239	168.2	1232	353.6
62	1258	116.5	1268	0.0	1270	97.7	1263	44.1
63	1261	0.0	1277	3.6	1271	0.0	1279	0.0
64	1286	0.0	1298	0.0	1294	0.0	1285	0.0
65	1310	180.5	1325	6.2	1334	29.3	1345	420.9
66	1326	36.6	1332	1.4	1348	23.4	1349	43.9
67	1327	0.0	1354	0.0	1350	0.0	1350	0.0
68	1347	80.6	1365	0.0	1368	0.0	1370	0.0
69	1351	0.0	1383	2.3	1368	113.0	1370	172.1
70	1370	0.0	1411	1.7	1408	0.0	1391	0.0
71	1395	0.0	1411	0.0	1417	0.0	1419	0.0
72	1405	14.1	1416	0.0	1420	2.7	1428	32.1
73	1407	8.2	1435	10.4	1439	31.7	1438	132.4
74	1439	0.0	1438	0.0	1449	0.0	1443	0.0
75	1440	10.9	1468	0.0	1453	0.0	1463	0.0
76	1445	0.0	1469	3.7	1455	17.1	1469	35.7
77	1483	0.6	1483	4.3	1486	35.6	1488	91.5
78	1507	12.4	1546	10.1	1515	12.5	1506	31.0
79	1513	0.0	1556	0.0	1529	0.0	1515	0.0
80	1542	0.0	1574	0.0	1547	0.0	1540	0.0
81	1544	110.5	1579	0.0	1549	29.5	1547	0.0
82	1545	0.0	1583	8.7	1555	0.0	1550	163.6
83	1576	154.0	1612	0.0	1571	228.7	1564	479.6
84	1588	0.0	1616	9.9	1597	0.0	1597	0.0
85	3004	0.0	3042	0.0	3065	2.6	3070	2.4
86	3004	86.0	3042	3.9	3065	0.0	3070	0.0
87	3006	3.4	3044	17.4	3071	0.4	3080	0.3
88	3007	0.0	3045	0.0	3071	0.0	3080	0.0
89	3015	0.0	3047	0.0	3073	0.1	3081	0.0
90	3015	37.0	3047	2.0	3073	0.0	3081	4.1
91	3026	42.8	3055	32.0	3077	4.0	3083	2.2
92	3027	0.0	3055	0.0	3077	0.0	3083	0.0
93	3032	0.0	3064	100.8	3087	17.5	3095	3.1
94	3033	288.9	3064	0.0	3087	0.0	3095	0.0
95	3042	324.1	3074	124.2	3100	17.3	3111	9.2
96	3043	0.0	3075	0.0	3100	0.0	3111	0.0