

Harmonic vibrational frequencies of tetracene ( $C_{18}H_{12}$ ) 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	57	0.2	55	0.6	54	1.0	51	1.9
2	87	0.0	90	0.0	88	0.0	87	0.0
3	150	0.0	147	0.0	142	0.0	135	0.0
4	160	1.6	160	1.1	160	0.6	162	0.0
5	191	0.0	191	0.0	191	0.0	187	0.0
6	285	0.2	266	0.6	255	1.7	240	2.0
7	298	0.0	301	0.0	300	0.0	301	0.0
8	298	0.0	311	0.0	310	0.0	308	0.0
9	309	0.0	315	0.0	319	0.0	316	0.0
10	345	0.0	374	0.0	378	0.0	380	0.0
11	440	0.4	442	0.0	438	27.9	418	54.9
12	455	3.7	464	22.2	441	0.1	435	0.8
13	462	0.0	468	0.0	454	6.9	440	0.2
14	463	6.5	472	1.4	466	0.0	462	0.0
15	502	0.0	500	0.0	490	0.0	464	0.0
16	542	0.0	512	0.0	497	0.0	472	0.0
17	552	31.3	556	8.7	546	0.0	523	0.0
18	562	0.0	561	0.0	552	0.6	547	9.4
19	616	0.1	611	1.8	615	0.5	618	0.0
20	626	0.0	629	0.0	626	0.0	619	1.3
21	630	3.8	640	1.4	630	0.1	622	2.0
22	702	0.0	718	0.0	702	0.0	683	0.0
23	703	0.0	733	0.0	743	0.0	730	0.0
24	716	72.3	735	2.1	744	3.4	740	0.0
25	730	0.0	742	0.0	744	0.0	744	6.8
26	731	0.0	746	84.2	754	0.0	747	0.0
27	737	37.5	754	0.0	755	0.0	765	111.5
28	742	0.0	763	0.0	758	101.7	768	0.0
29	771	0.0	776	0.0	781	0.0	786	0.0
30	773	0.0	833	0.0	850	0.0	850	0.0
31	777	0.0	841	0.0	853	0.0	870	0.0
32	803	0.0	843	0.0	870	0.0	890	0.0
33	823	105.2	850	0.0	882	0.0	894	0.0
34	832	0.0	884	0.0	897	0.0	921	0.0
35	839	0.0	899	0.0	908	0.0	931	0.3
36	853	0.0	905	81.8	934	56.2	938	0.0
37	885	0.0	916	0.0	935	0.9	967	27.4
38	887	21.5	935	1.9	944	0.0	984	0.0
39	888	0.0	959	0.0	979	0.0	997	0.0
40	925	0.0	961	10.0	982	12.9	1002	19.0
41	925	0.0	989	0.0	1017	0.0	1022	75.8
42	928	0.1	989	0.0	1017	0.0	1022	0.0
43	1012	0.0	996	3.6	1018	0.0	1037	0.0
44	1014	23.4	996	0.0	1018	1.9	1038	0.0
45	1104	7.4	1123	4.7	1123	0.8	1104	6.5
46	1110	0.0	1129	0.0	1127	0.0	1108	0.0
47	1157	3.5	1145	3.5	1180	24.6	1172	0.0
48	1161	0.0	1173	0.0	1188	0.0	1192	52.2
49	1170	0.0	1174	0.3	1189	139.8	1196	0.0
50	1182	49.4	1196	0.0	1192	0.0	1212	270.9
51	1198	0.6	1207	2.0	1215	0.0	1219	10.2
52	1209	0.0	1207	0.0	1220	0.0	1231	0.0

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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	1264	0.0	1278	0.0	1278	0.0	1272	0.0
54	1266	7.2	1283	11.6	1280	17.0	1277	174.2
55	1272	10.8	1292	0.8	1289	25.5	1289	29.0
56	1275	4.7	1292	4.8	1294	7.6	1302	11.3
57	1305	0.0	1335	0.0	1326	0.0	1326	0.0
58	1333	797.0	1337	8.2	1349	658.4	1351	584.6
59	1353	0.0	1370	0.0	1368	0.0	1358	0.0
60	1361	0.0	1391	0.0	1382	0.0	1397	0.0
61	1376	276.0	1391	0.5	1392	193.8	1415	20.0
62	1393	1.2	1399	1.6	1410	7.5	1432	0.0
63	1435	0.0	1449	0.0	1453	0.0	1443	142.2
64	1443	0.0	1451	0.0	1455	0.0	1449	0.0
65	1473	40.0	1469	3.8	1478	247.0	1458	0.0
66	1484	0.0	1514	0.0	1503	0.0	1495	515.9
67	1491	0.0	1525	0.0	1517	0.0	1497	60.7
68	1512	310.1	1536	2.8	1519	197.3	1511	0.0
69	1515	0.1	1562	1.1	1528	8.5	1537	0.0
70	1517	0.0	1599	0.0	1529	0.0	1539	485.4
71	1562	0.1	1613	0.0	1578	0.0	1553	0.0
72	1567	0.0	1626	9.4	1581	40.6	1561	126.8
73	3002	0.0	3039	0.0	3062	0.0	3066	0.0
74	3003	0.1	3041	1.9	3064	0.8	3068	0.6
75	3004	1.2	3042	16.9	3065	1.9	3069	4.8
76	3005	0.0	3044	0.0	3067	0.0	3070	0.0
77	3008	0.0	3044	0.0	3073	1.7	3083	0.0
78	3009	117.2	3045	31.8	3073	0.0	3083	2.9
79	3012	14.6	3048	1.3	3076	3.0	3085	0.3
80	3015	0.0	3049	0.0	3076	0.0	3085	0.0
81	3026	0.0	3064	0.0	3090	0.0	3099	0.0
82	3026	253.3	3064	81.5	3090	8.3	3099	6.4
83	3045	346.7	3078	120.0	3103	25.9	3110	10.9
84	3046	0.0	3079	0.0	3103	0.0	3110	0.0