

Harmonic vibrational frequencies of pentarylene ( $C_{50}H_{24}$ ) 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	14	0.0	14	0.1	14	0.2	13	0.7
2	21	0.0	19	0.0	21	0.0	23	0.0
3	29	0.0	28	0.0	33	0.0	34	0.0
4	36	0.0	36	0.0	35	0.0	37	0.0
5	37	0.0	36	0.0	46	0.0	53	0.0
6	41	0.0	40	0.0	57	0.0	63	0.4
7	64	0.0	62	0.1	63	0.2	66	0.5
8	66	0.1	66	0.1	66	0.2	68	0.0
9	113	0.1	112	0.2	117	0.0	118	0.0
10	114	0.0	114	0.0	119	0.4	123	0.5
11	146	0.0	146	0.0	147	0.0	148	0.0
12	146	0.0	146	0.0	147	0.0	148	0.0
13	157	0.0	152	0.0	154	0.0	156	0.0
14	166	0.0	159	0.0	164	0.0	166	0.2
15	175	0.0	171	0.0	171	0.0	170	0.0
16	177	6.6	175	9.6	173	13.9	171	18.6
17	206	0.0	211	0.0	211	0.0	209	0.0
18	207	0.0	212	0.0	213	0.0	214	0.0
19	232	0.7	232	0.1	233	0.0	234	0.0
20	242	0.0	247	0.0	244	0.0	242	0.0
21	255	0.6	249	0.8	248	0.8	247	0.8
22	278	0.0	285	0.0	282	0.0	280	0.0
23	286	1.7	287	4.7	285	0.0	280	0.0
24	290	0.0	291	0.0	288	28.1	290	38.1
25	306	0.0	306	0.0	306	0.0	306	0.0
26	326	0.0	333	0.0	330	0.0	325	1.1
27	334	1.2	339	1.1	332	1.1	328	0.0
28	372	0.0	373	0.0	369	0.0	365	0.0
29	372	0.0	373	0.0	374	0.0	375	0.0
30	375	1.5	373	0.0	376	0.1	377	0.8
31	410	0.0	411	0.0	412	0.0	413	0.0
32	411	0.0	419	0.0	419	0.0	414	0.0
33	421	0.0	420	0.0	421	0.0	423	0.0
34	423	0.1	425	0.0	422	0.2	424	0.8
35	439	2.6	440	3.9	439	10.2	437	24.3
36	449	0.0	449	0.0	448	0.0	439	0.0
37	451	0.0	457	0.0	449	0.0	448	0.0
38	476	0.0	463	0.2	460	0.0	453	0.0
39	477	0.4	463	0.0	460	1.2	453	3.9
40	484	0.0	471	0.2	474	0.0	476	0.0
41	484	0.0	474	0.0	476	0.9	481	2.1
42	485	0.1	485	0.0	484	1.9	483	10.9
43	496	0.0	485	0.4	497	0.0	490	0.0
44	498	0.0	501	0.0	499	0.0	498	0.0
45	506	0.0	507	0.0	499	0.0	507	0.0
46	511	46.8	515	0.4	514	7.3	515	57.8
47	532	0.0	535	0.0	534	0.0	533	0.0
48	532	0.0	538	0.0	535	0.0	533	0.0
49	538	0.0	542	1.0	540	2.2	536	0.0
50	541	67.1	545	16.9	541	0.0	537	3.6
51	542	0.2	546	0.0	545	6.6	546	2.8
52	549	0.0	560	0.0	557	0.2	554	0.7

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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	559	0.2	564	0.0	563	0.0	557	1.4
54	562	0.0	565	0.0	565	1.9	561	0.0
55	565	0.0	568	0.0	566	0.0	564	0.0
56	573	0.2	573	2.5	566	0.0	567	0.0
57	590	0.0	590	0.0	583	0.0	576	0.0
58	592	0.0	591	0.0	588	0.0	584	0.0
59	624	0.0	629	0.0	624	0.0	619	0.0
60	626	0.0	629	0.0	624	0.0	620	0.0
61	636	0.0	638	0.2	636	0.1	633	15.8
62	637	0.0	640	0.0	639	11.6	634	0.0
63	638	10.3	645	7.8	646	0.0	653	0.0
64	660	0.0	658	0.0	662	0.1	664	0.6
65	662	0.5	661	0.0	670	0.0	671	0.0
66	671	0.0	674	0.0	673	0.0	672	0.0
67	672	0.0	682	0.0	677	0.0	677	47.6
68	680	1.4	685	0.0	681	6.7	679	0.0
69	683	1.1	685	0.0	694	1.6	692	2.6
70	687	0.0	697	0.0	696	0.0	693	0.0
71	695	0.0	698	0.9	697	0.0	708	0.0
72	744	0.0	753	0.0	749	0.0	743	48.8
73	745	64.4	754	52.7	749	51.7	743	0.0
74	746	0.0	754	0.7	753	0.2	751	0.0
75	746	0.0	762	0.0	768	0.0	767	0.0
76	751	0.0	762	0.0	771	0.0	776	0.0
77	767	0.0	771	0.0	772	0.0	782	0.0
78	770	1.3	777	0.1	775	0.1	784	0.0
79	781	0.0	789	129.2	787	38.5	789	23.3
80	785	12.2	791	0.0	791	0.0	793	0.0
81	792	0.0	793	0.0	793	0.0	793	0.0
82	794	116.3	797	13.3	798	11.2	798	11.3
83	795	272.8	801	0.0	802	0.0	802	0.0
84	796	0.0	809	5.2	809	1.5	808	0.0
85	798	0.0	815	0.0	813	0.0	810	0.0
86	799	0.0	818	0.0	815	308.2	814	310.2
87	799	0.0	818	304.6	817	0.0	814	0.0
88	806	8.5	819	0.0	821	0.0	823	0.0
89	811	0.0	824	0.0	827	0.0	830	0.0
90	812	0.0	824	0.0	828	0.0	833	0.0
91	813	0.1	826	0.0	829	0.0	834	0.0
92	817	0.0	831	0.4	833	1.4	835	5.6
93	828	0.0	838	0.0	840	1.2	844	1.8
94	829	12.7	838	0.0	840	0.0	844	0.0
95	841	0.0	873	18.4	873	1.8	866	16.2
96	841	0.0	877	2.3	876	5.3	879	0.5
97	864	1.4	882	0.0	903	0.0	927	0.0
98	864	0.0	882	0.0	903	0.0	927	0.0
99	872	0.1	902	0.5	923	2.6	948	4.8
100	872	40.4	902	0.0	923	0.0	948	0.0
101	908	0.0	932	0.0	948	0.0	952	0.0
102	916	0.0	939	0.0	951	0.0	961	0.0
103	920	0.0	941	0.0	956	0.0	967	0.0
104	926	0.1	944	0.0	961	0.0	971	0.0
105	933	0.0	946	0.0	963	0.0	978	0.0
106	937	0.0	950	0.0	964	0.0	979	0.1

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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. ( $\text{km mol}^{-1}$ )
107	943	0.0	954	0.0	970	0.0	983	14.9
108	949	0.0	965	0.0	972	0.0	986	0.0
109	949	0.0	971	0.0	987	0.0	986	0.0
110	956	2.7	971	0.0	987	0.0	1004	0.0
111	956	0.0	980	2.5	989	3.3	1005	0.0
112	961	0.0	980	0.0	996	1.0	1014	0.2
113	988	6.5	995	1.3	996	0.0	1014	0.0
114	1009	109.5	1011	28.4	1016	17.6	1021	76.2
115	1026	0.0	1034	0.0	1030	0.0	1024	0.0
116	1045	5.7	1051	2.4	1051	0.1	1048	0.8
117	1058	0.0	1061	0.0	1063	0.0	1063	0.0
118	1069	0.0	1069	0.0	1077	0.0	1081	0.0
119	1082	1.8	1081	0.5	1085	0.6	1085	0.5
120	1095	24.6	1096	0.0	1100	1.8	1104	43.3
121	1095	0.0	1096	2.5	1101	0.0	1104	0.0
122	1129	0.0	1141	0.0	1135	0.0	1127	0.0
123	1142	0.5	1148	2.9	1149	6.4	1147	9.1
124	1154	0.0	1162	0.0	1160	0.0	1155	0.0
125	1160	27.9	1163	0.0	1169	1.9	1160	0.0
126	1161	0.0	1164	0.8	1169	0.0	1161	3.0
127	1164	1.4	1177	0.0	1170	0.3	1172	0.9
128	1165	0.0	1178	0.0	1171	0.0	1174	0.0
129	1177	0.0	1182	0.0	1185	0.0	1187	0.0
130	1184	43.9	1186	11.6	1189	69.0	1190	489.9
131	1193	0.0	1200	0.0	1202	0.0	1205	0.2
132	1194	0.2	1201	0.2	1203	0.0	1205	0.0
133	1203	1.4	1206	0.6	1212	3.9	1217	10.8
134	1207	115.3	1214	7.6	1220	148.0	1226	490.1
135	1213	0.0	1215	0.0	1222	0.0	1227	0.0
136	1214	0.0	1220	2.6	1223	0.0	1229	0.0
137	1218	0.0	1220	0.0	1227	31.7	1233	23.6
138	1226	19.3	1231	0.0	1237	0.0	1235	227.5
139	1227	0.0	1241	7.5	1241	78.2	1241	0.0
140	1241	0.0	1243	0.0	1246	0.0	1265	0.0
141	1253	1594.5	1274	5.5	1260	1669.5	1276	5331.1
142	1255	34.4	1276	0.0	1269	25.7	1277	14.7
143	1277	0.0	1283	2.1	1286	0.0	1293	0.0
144	1282	0.0	1284	10.0	1293	0.0	1295	0.0
145	1290	0.0	1290	2.8	1298	0.0	1301	168.2
146	1290	14.7	1291	0.0	1299	7.0	1302	0.0
147	1295	6.3	1298	0.0	1307	75.0	1312	46.1
148	1303	30.6	1307	0.0	1312	70.8	1314	49.7
149	1304	0.0	1309	0.0	1314	0.0	1331	0.0
150	1311	69.7	1311	17.1	1319	0.0	1337	0.0
151	1314	0.0	1318	1.2	1322	0.0	1339	0.0
152	1314	0.0	1321	0.3	1331	0.0	1341	12.6
153	1326	1.2	1322	0.0	1338	1.5	1351	113.4
154	1337	89.6	1339	2.9	1349	4.1	1356	0.3
155	1337	0.0	1340	0.0	1351	0.0	1357	0.0
156	1339	1.1	1347	13.0	1354	0.0	1360	0.0
157	1340	0.0	1353	0.0	1355	0.6	1365	576.4
158	1344	173.0	1354	8.1	1356	88.0	1368	0.0
159	1352	0.0	1356	0.0	1359	0.0	1378	0.0
160	1364	0.0	1362	0.0	1370	0.0	1382	0.2

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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. ( $\text{km mol}^{-1}$ )
161	1380	89.6	1386	198.2	1388	176.4	1390	85.9
162	1397	0.2	1399	8.9	1407	1.0	1413	9.3
163	1403	0.0	1403	0.0	1411	0.0	1417	0.0
164	1422	0.0	1422	0.0	1430	0.0	1424	0.0
165	1423	0.0	1427	1.3	1436	0.0	1442	0.0
166	1434	12.7	1447	0.0	1441	14.6	1444	0.0
167	1438	2.9	1448	21.4	1449	0.0	1445	3.1
168	1444	0.0	1448	0.0	1449	1.0	1452	30.6
169	1445	10.7	1453	0.0	1453	48.8	1456	7.1
170	1446	0.0	1457	0.7	1453	0.0	1458	0.0
171	1448	1.7	1460	2.7	1458	4.9	1458	32.7
172	1448	0.0	1465	0.0	1460	0.0	1461	0.0
173	1486	35.6	1494	26.8	1491	16.6	1493	0.0
174	1491	0.0	1496	0.0	1493	0.0	1495	33.5
175	1504	0.7	1505	0.0	1506	0.0	1509	11.9
176	1517	0.0	1518	0.0	1520	0.0	1509	30.6
177	1522	810.3	1523	0.0	1529	982.3	1518	0.0
178	1527	0.0	1531	0.3	1532	0.0	1527	0.0
179	1534	905.9	1545	21.1	1532	36.7	1540	167.1
180	1537	0.0	1558	0.0	1542	0.0	1548	0.0
181	1540	0.5	1561	50.5	1543	3.6	1549	12.9
182	1543	0.8	1564	37.2	1549	40.1	1550	4178.0
183	1548	0.0	1565	0.0	1553	0.0	1555	0.0
184	1555	0.0	1567	0.0	1555	0.0	1557	0.0
185	1562	0.0	1576	0.4	1565	0.0	1557	1.0
186	1563	4.3	1577	20.0	1567	5.1	1561	0.0
187	1567	0.3	1581	0.0	1568	194.0	1565	0.0
188	1569	0.0	1581	49.2	1568	0.0	1573	13.2
189	1575	8.6	1583	0.0	1571	21.6	1580	992.7
190	1578	77.3	1589	0.0	1586	0.9	1584	22.4
191	1578	0.0	1599	0.0	1586	0.0	1585	0.0
192	1590	0.0	1599	10.5	1588	0.0	1596	0.0
193	3029	0.0	3050	0.0	3066	0.0	3077	0.0
194	3029	48.1	3050	8.9	3066	1.0	3077	0.0
195	3031	86.1	3052	11.3	3068	1.4	3079	0.0
196	3031	0.0	3052	0.0	3068	0.0	3079	0.0
197	3050	0.0	3069	0.0	3084	0.0	3095	0.0
198	3050	59.2	3069	29.0	3084	9.2	3095	12.1
199	3053	738.6	3070	439.6	3084	196.7	3095	0.4
200	3053	0.0	3071	0.0	3084	0.0	3096	0.0
201	3060	1.0	3075	0.0	3089	3.7	3099	28.3
202	3060	0.0	3075	8.5	3089	0.0	3099	0.0
203	3064	0.0	3079	4.6	3093	5.2	3104	0.0
204	3064	0.0	3079	0.0	3093	0.0	3104	1.6
205	3070	0.0	3084	0.0	3098	0.0	3108	0.0
206	3070	0.4	3085	5.8	3098	14.3	3108	8.1
207	3080	3.4	3091	8.6	3103	7.5	3112	2.2
208	3081	0.0	3091	0.0	3103	0.0	3112	0.0
209	3087	0.0	3097	0.0	3109	0.0	3119	0.0
210	3088	21.5	3097	21.1	3109	22.9	3119	7.1
211	3091	50.9	3102	28.7	3115	14.0	3125	2.9
212	3092	0.0	3102	0.0	3115	0.0	3125	0.0
213	3095	0.0	3106	0.0	3119	0.0	3129	0.0
214	3096	81.0	3106	54.2	3119	59.4	3129	24.7

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	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. ( $\text{km mol}^{-1}$ )
215	3099	240.0	3109	143.5	3123	79.3	3132	36.8
216	3100	0.0	3110	0.0	3123	0.0	3133	0.0