

Harmonic vibrational frequencies of circumpyrene ($C_{42}H_{16}$) 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	44	0.1	44	0.2	45	0.6	45	1.2
2	53	0.0	54	0.0	55	0.0	54	0.0
3	78	0.8	74	2.8	74	5.8	71	10.0
4	97	0.0	97	0.0	97	0.0	96	0.0
5	114	0.0	113	0.0	113	0.0	113	0.0
6	166	0.0	169	0.0	167	0.0	165	0.0
7	171	0.0	171	0.0	168	0.0	166	0.0
8	181	0.0	180	0.0	177	0.0	173	0.0
9	190	0.3	189	0.1	191	0.0	190	0.4
10	244	1.5	247	1.0	245	1.8	241	2.6
11	252	0.0	252	0.0	252	0.0	252	0.0
12	253	25.0	256	3.4	255	1.6	253	1.1
13	270	0.0	271	0.0	272	0.0	272	0.0
14	280	0.0	282	0.0	279	0.0	274	0.0
15	287	0.0	289	0.0	286	0.0	284	0.0
16	309	3.8	316	6.2	313	0.0	304	0.0
17	324	0.0	321	0.0	319	6.9	319	7.7
18	331	8.0	330	6.8	330	9.2	331	6.8
19	353	0.4	358	0.0	355	0.0	349	0.0
20	361	0.0	361	0.5	359	0.0	350	0.0
21	363	0.0	362	0.0	362	2.0	363	0.0
22	363	0.0	365	0.0	363	0.0	364	4.0
23	363	0.0	368	0.0	371	0.0	371	0.0
24	372	0.0	374	0.0	372	0.0	373	0.0
25	379	0.0	379	1.4	377	0.0	374	0.5
26	418	0.0	426	0.0	425	0.0	426	0.0
27	432	5.6	436	0.0	437	1.4	437	6.9
28	457	0.0	457	0.0	458	0.0	452	0.0
29	466	0.0	468	0.0	461	0.0	458	0.0
30	469	0.0	477	0.0	468	0.0	458	0.0
31	482	0.0	483	0.0	481	0.0	478	0.0
32	520	0.0	522	0.0	517	0.0	510	0.0
33	520	0.7	523	1.4	521	0.0	519	0.0
34	520	0.0	524	0.0	522	4.7	521	13.1
35	527	1.4	529	0.1	527	0.1	524	0.8
36	544	0.6	544	0.0	543	2.8	541	13.9
37	548	4.3	553	0.0	550	0.0	547	0.0
38	549	0.0	554	2.1	552	0.0	550	0.1
39	553	0.0	555	0.0	553	0.3	550	0.0
40	563	0.0	563	0.0	562	0.0	560	0.0
41	569	4.2	572	5.3	574	8.4	576	10.7
42	583	0.0	583	0.0	583	0.0	580	0.0
43	586	0.0	594	0.0	588	0.0	581	0.0
44	602	9.0	602	1.4	604	0.3	605	0.1
45	604	0.0	616	0.0	617	2.9	615	0.0
46	613	9.1	617	1.2	618	0.0	616	24.7
47	619	0.0	623	0.0	619	0.0	622	22.9
48	620	13.7	625	17.6	623	20.3	625	0.0
49	626	0.0	626	0.0	628	0.0	629	0.0
50	630	0.1	631	0.6	631	0.3	631	3.0
51	639	0.0	638	0.0	638	0.0	637	0.0
52	681	5.2	683	0.7	684	0.0	684	2.8

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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	695	0.0	694	0.0	695	0.0	695	0.1
54	701	0.0	704	0.0	702	0.0	699	0.0
55	703	0.0	707	10.7	708	10.2	704	0.0
56	703	8.3	709	0.0	709	0.0	711	10.1
57	709	0.0	715	0.0	709	0.0	714	0.0
58	728	0.0	730	0.0	729	0.0	727	0.0
59	738	0.0	742	0.0	736	0.0	732	0.0
60	745	0.0	747	3.4	747	1.6	746	0.0
61	755	0.0	765	0.0	765	0.0	763	0.0
62	761	0.0	772	0.0	768	0.0	768	0.0
63	764	9.7	775	0.0	771	0.0	771	0.0
64	764	0.0	777	0.0	776	0.8	772	0.0
65	765	0.0	780	7.3	777	0.0	775	0.0
66	774	0.0	784	0.0	787	0.0	797	0.0
67	774	0.0	789	0.0	796	0.0	803	0.0
68	784	7.8	796	23.7	807	41.2	821	52.4
69	793	0.0	808	0.0	818	0.0	829	0.0
70	801	0.0	831	0.0	831	0.0	829	0.0
71	810	10.4	832	0.0	845	0.0	847	40.9
72	827	0.0	838	28.5	850	10.7	847	0.0
73	839	0.0	852	1.3	850	35.7	854	1.7
74	847	0.0	853	0.0	851	0.0	860	0.0
75	848	0.5	857	8.8	856	0.0	864	48.0
76	849	0.0	884	0.0	902	0.0	907	0.4
77	852	0.0	890	0.0	907	0.9	920	0.0
78	853	0.2	896	0.0	909	0.0	921	0.0
79	857	206.9	900	176.1	914	0.0	925	0.0
80	903	0.0	904	0.0	918	0.0	931	0.0
81	912	0.0	912	0.0	919	165.1	938	0.0
82	916	0.0	918	0.0	920	0.0	943	148.5
83	929	0.0	960	0.0	969	11.4	965	15.3
84	930	0.0	960	0.0	977	0.0	993	0.0
85	940	0.0	971	3.0	978	0.0	996	0.0
86	941	0.0	972	0.0	986	0.0	997	0.0
87	946	0.2	974	0.2	987	0.0	1000	0.0
88	947	0.0	976	0.0	992	0.0	1009	0.0
89	964	0.0	977	0.0	993	0.0	1010	0.0
90	1017	0.0	1024	0.0	1022	0.0	1020	0.0
91	1039	0.0	1047	0.0	1047	0.0	1044	0.0
92	1060	2.2	1057	1.6	1066	2.1	1072	21.1
93	1077	0.0	1083	0.0	1088	0.0	1090	0.0
94	1085	0.4	1090	0.3	1094	28.0	1092	92.6
95	1095	4.7	1101	0.0	1104	1.9	1104	18.5
96	1135	10.9	1143	0.1	1145	2.0	1145	0.7
97	1151	0.0	1161	0.0	1162	0.0	1164	0.0
98	1155	0.0	1163	0.0	1168	0.0	1170	0.0
99	1157	6.4	1163	0.0	1170	53.1	1173	135.8
100	1164	3.4	1167	5.2	1178	0.4	1183	27.4
101	1171	0.0	1182	18.6	1184	0.0	1185	0.0
102	1179	74.7	1183	0.0	1188	14.1	1192	0.0
103	1191	0.0	1194	0.0	1198	0.0	1202	0.0
104	1206	3.8	1210	3.9	1213	53.7	1214	189.8
105	1220	0.0	1223	0.0	1220	0.0	1223	0.0
106	1223	143.0	1224	9.9	1228	17.2	1229	25.0

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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})
107	1228	0.0	1233	0.0	1234	0.0	1239	0.0
108	1229	0.0	1237	0.0	1241	0.0	1247	0.0
109	1244	4.9	1248	18.6	1250	312.7	1250	279.0
110	1248	304.2	1265	1.6	1253	16.3	1255	0.0
111	1265	0.0	1279	0.0	1269	0.0	1255	41.6
112	1286	0.0	1291	0.0	1295	0.0	1295	0.0
113	1302	127.6	1305	1.7	1309	0.0	1298	0.0
114	1304	0.0	1312	0.0	1316	38.2	1317	5.4
115	1311	39.9	1316	18.4	1317	8.0	1324	0.4
116	1314	128.8	1321	4.8	1332	71.1	1339	435.8
117	1319	0.0	1332	0.0	1334	0.0	1342	0.0
118	1336	0.0	1356	0.0	1353	0.0	1357	0.0
119	1343	39.2	1362	6.7	1358	86.2	1366	420.7
120	1344	216.0	1365	0.0	1360	85.0	1366	5.3
121	1353	0.0	1367	1.2	1369	0.0	1369	0.0
122	1359	0.0	1368	0.0	1371	0.0	1370	0.0
123	1366	0.0	1382	0.0	1380	0.0	1374	0.0
124	1379	12.9	1394	5.6	1393	0.1	1389	0.8
125	1381	0.0	1396	2.7	1394	4.3	1390	0.7
126	1388	5.8	1397	0.1	1399	0.0	1403	0.0
127	1392	39.8	1398	0.0	1402	0.6	1408	0.0
128	1392	6.8	1401	0.0	1411	0.0	1408	6.0
129	1399	0.0	1411	5.8	1413	4.3	1416	0.5
130	1412	10.2	1419	1.5	1423	0.2	1426	3.3
131	1419	0.0	1426	0.0	1431	0.0	1433	0.0
132	1420	0.0	1435	0.0	1432	0.0	1435	0.0
133	1435	0.0	1454	0.9	1448	0.0	1450	0.0
134	1440	0.0	1455	0.0	1451	184.7	1455	421.8
135	1447	45.8	1463	0.0	1454	0.0	1458	0.0
136	1454	50.6	1466	0.1	1465	9.4	1461	94.5
137	1458	1.3	1472	6.1	1471	3.2	1470	60.4
138	1469	14.0	1480	0.1	1475	6.8	1477	6.3
139	1481	0.0	1485	0.0	1486	0.0	1486	0.0
140	1487	0.2	1501	2.2	1495	14.6	1502	0.2
141	1502	0.0	1504	0.0	1504	0.0	1503	0.0
142	1507	0.0	1534	0.0	1516	0.0	1510	0.0
143	1541	0.0	1555	0.7	1548	0.0	1540	0.0
144	1543	5.9	1563	0.0	1554	38.6	1548	0.3
145	1549	0.0	1571	5.1	1555	5.5	1549	263.9
146	1559	7.2	1584	1.1	1557	0.0	1561	0.0
147	1565	98.0	1585	0.0	1566	23.1	1564	0.0
148	1574	0.0	1591	0.0	1572	0.0	1564	4.6
149	1584	188.8	1596	0.0	1577	581.0	1578	898.7
150	1585	152.5	1604	29.4	1589	9.2	1586	136.8
151	1588	0.0	1609	14.8	1592	0.0	1588	0.0
152	1598	0.0	1612	0.0	1597	0.0	1596	0.0
153	3016	0.0	3042	0.0	3060	0.0	3068	0.0
154	3016	1.2	3042	3.0	3060	2.0	3068	1.5
155	3019	16.7	3043	3.7	3061	14.6	3068	0.1
156	3019	0.0	3044	0.0	3061	0.0	3069	0.0
157	3020	0.0	3044	0.0	3065	0.0	3076	0.0
158	3020	96.8	3045	17.0	3065	1.0	3076	0.0
159	3025	46.6	3045	52.7	3065	7.6	3077	0.3
160	3026	0.0	3046	0.0	3066	0.0	3077	0.0

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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})
161	3027	0.0	3046	0.0	3066	0.0	3077	0.0
162	3027	23.0	3047	0.7	3066	0.0	3077	1.2
163	3043	0.3	3064	8.7	3082	18.7	3091	4.2
164	3044	0.0	3064	0.0	3082	0.0	3091	0.0
165	3044	0.0	3065	0.0	3082	0.0	3092	0.0
166	3045	376.6	3065	169.2	3082	45.4	3092	1.1
167	3045	416.0	3066	218.4	3084	87.1	3094	8.9
168	3046	0.0	3066	0.0	3084	0.0	3094	0.0