

Harmonic vibrational frequencies of triphenylene ($C_{18}H_{12}$) 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	27	0.0	50	0.0	42	0.0	42	0.0
2	58	0.0	50	0.0	56	0.0	43	0.0
3	79	0.0	108	0.0	92	0.0	71	0.0
4	121	0.5	119	2.1	117	4.8	117	8.7
5	211	587.1	256	0.3	117	164.0	220	44.3
6	254	0.0	256	0.3	248	0.0	222	43.5
7	255	4.3	269	0.0	255	0.0	235	0.0
8	258	0.0	269	0.0	256	0.3	235	0.0
9	270	180.0	403	0.8	307	29.8	362	65.2
10	391	0.0	403	0.8	401	0.0	362	64.1
11	401	0.2	411	0.0	401	0.5	383	5.0
12	404	8.0	424	4.2	402	5.0	391	0.0
13	412	0.5	428	0.0	413	0.1	392	0.0
14	429	0.4	428	0.0	422	0.4	411	0.0
15	493	1085.3	542	0.0	494	0.0	460	0.0
16	514	0.0	542	0.0	522	0.6	485	0.0
17	517	1.1	556	0.0	530	0.0	486	0.0
18	553	2.3	573	0.0	558	1.4	519	128.2
19	561	0.0	615	0.0	564	1.0	519	128.6
20	601	8.6	631	5.2	603	2.8	557	0.0
21	620	2.9	631	5.2	619	10.6	588	0.0
22	651	265.1	699	0.0	673	242.8	667	0.0
23	660	0.0	710	0.0	683	2.9	687	0.0
24	681	1.1	710	0.0	686	13.5	687	0.0
25	683	0.6	743	180.0	708	0.0	743	0.0
26	693	152.4	766	0.0	745	0.0	750	77.4
27	708	0.0	773	0.0	750	179.7	750	78.4
28	717	2.6	773	0.0	772	0.9	752	215.4
29	729	0.0	776	0.0	777	0.0	769	0.0
30	766	10.8	776	0.0	781	4.9	769	0.0
31	774	0.0	855	0.0	860	0.0	867	0.0
32	781	6.4	855	0.0	867	1.9	868	0.0
33	789	417.7	867	0.0	876	0.0	873	0.0
34	801	0.0	932	0.0	904	138.4	963	231.0
35	847	0.0	932	0.0	956	0.0	963	224.1
36	868	4.9	946	1.9	960	0.0	974	0.0
37	887	1.6	978	0.0	974	30.6	974	0.0
38	906	0.0	985	0.0	974	2.1	987	3.3
39	923	0.1	985	0.0	1006	0.0	989	189.7
40	924	0.0	996	1.7	1010	0.2	990	192.8
41	970	40.8	996	1.7	1010	1.0	1005	0.0
42	1002	0.5	1013	0.0	1013	0.0	1018	0.0
43	1007	29.0	1054	3.5	1024	0.9	1024	0.0
44	1021	0.2	1054	3.5	1044	7.7	1024	0.0
45	1046	0.4	1062	0.0	1060	2.2	1030	50.3
46	1052	18.8	1108	0.2	1067	0.0	1030	48.9
47	1080	8.3	1108	0.2	1097	6.9	1039	0.1
48	1081	58.7	1153	0.0	1105	2.7	1100	21.2
49	1132	196.0	1185	0.3	1156	8.1	1100	20.4
50	1151	283.9	1185	0.3	1189	231.8	1145	0.0
51	1163	21.1	1198	0.0	1192	14.5	1199	0.0
52	1173	4.6	1222	0.0	1203	5.5	1228	11.6

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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	1212	92.8	1253	3.3	1242	46.7	1229	12.0
54	1238	214.9	1253	3.3	1272	51.2	1261	0.0
55	1267	5.8	1291	1.8	1274	24.6	1298	0.4
56	1279	497.3	1291	1.8	1302	9.7	1300	45.0
57	1281	77.0	1304	0.0	1307	19.4	1300	45.8
58	1294	132.9	1323	0.0	1330	1.2	1327	0.0
59	1308	11.4	1337	0.7	1336	310.9	1331	101.2
60	1357	21.5	1337	0.7	1357	10.5	1332	102.3
61	1366	26.5	1440	23.5	1374	1.3	1391	3.1
62	1401	92.6	1440	23.5	1434	137.3	1393	3.5
63	1417	9.0	1441	0.0	1434	22.7	1444	0.1
64	1439	7.4	1460	0.0	1443	37.3	1448	0.6
65	1445	41.2	1497	12.6	1455	42.7	1455	118.4
66	1473	9.1	1497	12.6	1485	15.4	1456	117.6
67	1490	218.2	1544	0.0	1511	0.1	1480	3.6
68	1503	77.6	1565	0.2	1520	103.0	1480	3.5
69	1504	57.8	1565	0.2	1537	14.9	1500	0.0
70	1526	7.3	1596	0.5	1538	223.7	1504	0.0
71	1558	15.3	1596	0.5	1574	97.8	1556	3.3
72	1568	68.1	1601	0.0	1575	10.0	1556	2.7
73	3003	150.8	3053	0.0	3084	0.1	3097	0.0
74	3004	0.2	3054	2.6	3086	0.4	3097	0.6
75	3007	41.6	3054	2.6	3086	1.4	3098	0.7
76	3025	56.5	3068	52.1	3097	3.4	3106	11.6
77	3030	112.0	3068	52.1	3098	4.3	3106	11.5
78	3036	28.7	3072	0.0	3100	0.1	3108	0.0
79	3044	7.1	3084	0.0	3108	1.7	3120	0.0
80	3052	51.0	3089	1.3	3114	8.1	3122	0.0
81	3056	3.7	3089	1.3	3115	1.0	3124	0.0
82	3071	154.7	3105	61.8	3124	9.7	3142	1.2
83	3071	102.2	3105	61.9	3134	13.8	3142	0.9
84	3076	4.5	3108	0.0	3136	3.0	3144	0.3