

Harmonic vibrational frequencies of biphenylene ($C_{12}H_8$) 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	101	0.8	100	2.5	96	5.0	87	7.8
2	150	0.0	149	0.0	129	0.0	109	0.0
3	211	1.7	204	0.8	211	1.8	220	1.6
4	305	0.0	314	0.0	282	0.0	243	0.0
5	384	0.0	379	2.7	371	2.7	349	0.0
6	385	8.8	386	0.0	396	0.0	360	2.4
7	390	0.0	424	0.0	409	0.0	400	0.0
8	398	0.0	452	0.0	456	0.0	402	0.0
9	545	0.0	552	0.0	499	0.0	493	0.0
10	560	0.0	577	0.0	555	0.0	551	0.0
11	589	0.0	611	0.0	605	0.0	587	42.2
12	610	0.1	622	3.8	608	29.4	606	0.0
13	653	0.0	710	0.0	687	0.0	663	0.0
14	667	0.0	719	0.3	713	2.2	701	6.4
15	672	98.8	739	125.4	754	150.2	725	0.0
16	702	0.0	751	0.0	756	0.0	739	0.0
17	738	0.0	759	0.0	757	0.0	762	173.6
18	741	0.0	784	0.0	781	0.0	809	0.0
19	772	0.0	874	0.0	886	0.0	895	0.0
20	775	0.0	888	0.0	897	0.0	905	0.0
21	857	8.7	921	7.0	951	65.5	912	150.9
22	860	0.0	928	0.0	971	0.0	921	0.0
23	890	0.0	958	15.2	974	4.5	927	14.3
24	891	0.0	976	0.0	977	0.0	979	0.0
25	928	177.4	977	0.0	980	0.2	1011	3.7
26	960	0.0	986	0.0	993	0.0	1011	0.0
27	965	31.3	997	0.0	1016	0.0	1043	0.0
28	984	0.0	1017	0.0	1017	0.0	1045	0.0
29	1044	0.1	1052	0.8	1064	2.0	1067	9.3
30	1087	3.4	1082	0.0	1103	0.0	1127	0.0
31	1088	0.0	1089	0.0	1117	0.0	1136	0.0
32	1090	0.0	1124	9.2	1142	17.3	1143	7.2
33	1146	1.5	1175	7.0	1187	9.0	1196	5.9
34	1171	0.0	1183	0.0	1198	0.0	1218	0.0
35	1250	33.3	1270	20.2	1287	1.0	1296	0.0
36	1272	85.8	1271	1.0	1298	12.7	1317	11.4
37	1286	0.0	1300	0.0	1303	0.0	1345	55.0
38	1364	18.3	1399	0.0	1391	0.0	1383	0.0
39	1373	0.0	1421	36.2	1399	2.9	1391	45.5
40	1379	61.1	1445	8.3	1456	0.0	1442	5.4
41	1442	0.0	1448	0.0	1470	24.9	1450	0.0
42	1446	0.1	1458	0.0	1471	0.0	1460	0.0
43	1454	0.0	1574	1.1	1484	0.2	1473	490.5
44	1491	129.8	1579	1.0	1513	246.4	1491	49.2
45	1539	0.0	1602	0.0	1531	0.0	1511	0.0
46	1620	0.0	1661	0.0	1638	0.0	1631	0.0
47	2985	10.9	3051	0.0	3086	0.0	3086	2.9
48	2986	0.0	3051	1.2	3087	0.0	3086	0.0
49	2993	2.3	3064	29.9	3097	0.0	3093	62.0
50	2996	0.0	3065	0.0	3097	0.0	3093	0.0
51	3009	0.0	3075	0.0	3110	0.0	3112	0.0
52	3010	330.2	3076	67.1	3111	0.8	3112	18.8

continued on next page

Table 1 - continued from previous page

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	3028	320.1	3082	56.1	3113	1.0	3112	85.3
54	3031	0.0	3084	0.0	3113	0.0	3113	0.0