

Harmonic vibrational frequencies of bisanthene (C₂₈H₁₄) 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	36	0.0	31	0.0	40	0.0	43	0.0
2	82	0.1	79	0.0	82	0.1	79	0.1
3	87	0.0	81	0.1	93	0.0	99	12.8
4	106	1.0	105	3.5	103	7.3	99	0.0
5	146	0.0	150	0.0	148	0.0	145	0.0
6	177	0.0	173	0.0	183	0.0	187	0.0
7	243	0.0	238	0.0	232	0.0	223	0.0
8	249	0.0	252	0.0	250	0.0	246	0.0
9	271	0.3	278	0.1	277	1.6	273	2.1
10	281	0.7	278	0.0	283	0.4	284	2.0
11	305	0.0	307	0.0	310	0.0	312	0.0
12	307	0.0	307	0.0	310	0.0	315	0.0
13	317	15.6	318	8.0	316	7.6	317	0.1
14	332	0.0	329	0.0	324	0.0	317	0.0
15	335	0.0	331	0.0	330	0.0	325	0.0
16	361	0.0	361	0.0	362	0.0	362	0.0
17	393	1.4	407	1.0	403	2.2	400	3.0
18	416	0.0	416	0.0	418	0.0	418	0.0
19	455	0.8	456	1.3	453	1.2	449	1.7
20	497	2.2	486	0.0	484	0.0	478	0.0
21	500	0.0	500	0.0	493	0.0	480	0.0
22	514	0.0	500	0.1	498	0.0	489	0.0
23	516	0.0	507	0.0	501	0.1	498	0.0
24	519	0.0	518	0.0	512	0.0	500	13.7
25	522	0.0	524	0.0	517	0.0	513	0.0
26	537	4.4	539	9.4	532	13.6	525	20.8
27	562	0.6	561	0.9	558	5.6	554	17.7
28	586	0.0	586	0.0	583	4.1	573	8.9
29	587	0.0	589	0.7	584	0.0	580	0.0
30	620	0.0	626	0.0	619	0.0	612	0.0
31	624	0.0	629	0.0	631	0.0	629	0.0
32	630	0.0	632	0.0	632	1.2	631	5.9
33	631	2.2	635	2.2	633	0.0	633	0.0
34	641	0.0	644	0.0	644	0.0	644	0.0
35	652	0.0	654	0.0	657	0.0	658	0.0
36	665	7.0	665	11.7	667	12.1	671	1.2
37	698	0.0	710	4.3	710	2.0	706	19.5
38	708	12.7	723	0.0	724	0.0	711	0.0
39	722	0.0	734	0.0	724	0.0	723	0.0
40	728	99.5	754	116.6	756	78.0	750	60.5
41	732	0.0	759	0.0	768	0.0	771	0.0
42	759	8.2	773	8.6	774	0.1	773	0.0
43	763	0.0	776	7.3	777	0.0	773	15.4
44	764	13.6	780	0.0	783	68.9	796	101.6
45	769	0.0	788	0.0	795	0.0	804	0.0
46	777	0.0	806	0.0	814	0.0	825	0.0
47	794	0.0	811	0.0	821	0.0	831	0.0
48	804	78.0	868	78.9	893	0.0	893	0.0
49	815	0.0	871	0.0	893	51.3	895	5.5
50	820	0.0	887	0.0	895	2.9	920	0.1
51	833	0.0	891	0.5	896	0.0	924	0.0
52	845	0.0	893	0.0	918	0.0	926	24.9

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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	849	44.2	894	0.0	921	7.6	948	0.0
54	884	39.9	901	0.0	924	0.0	952	0.0
55	892	0.0	905	15.6	935	0.0	955	0.0
56	914	19.0	921	13.4	938	16.4	974	0.0
57	930	0.0	947	0.0	953	0.0	977	19.9
58	932	0.0	973	0.0	998	0.0	1000	1.3
59	936	0.0	975	0.0	1000	0.0	1009	0.0
60	936	3.1	976	0.0	1001	0.0	1019	0.0
61	949	0.0	977	3.2	1001	0.0	1022	0.0
62	992	1.2	996	0.9	1003	1.1	1023	0.0
63	1000	0.0	1000	0.0	1008	0.0	1025	0.2
64	1071	0.0	1070	0.7	1078	0.0	1076	0.0
65	1073	0.8	1074	0.0	1079	1.0	1083	0.8
66	1080	0.0	1084	0.0	1091	0.0	1090	0.0
67	1088	25.5	1088	6.5	1095	0.5	1092	9.3
68	1121	0.0	1122	0.0	1133	0.0	1140	0.0
69	1141	0.0	1147	0.0	1154	0.0	1156	0.0
70	1157	10.4	1170	6.9	1170	1.9	1172	11.9
71	1174	0.0	1177	0.0	1190	0.0	1202	0.0
72	1183	19.9	1182	1.8	1196	71.6	1207	115.2
73	1189	10.3	1193	2.1	1206	2.2	1216	2.4
74	1199	0.0	1202	0.0	1213	0.0	1222	0.0
75	1207	0.7	1209	0.0	1222	0.0	1222	6.4
76	1208	0.0	1219	0.6	1223	0.3	1231	0.0
77	1253	0.0	1267	0.0	1267	0.0	1262	620.2
78	1263	8.7	1273	14.9	1272	13.6	1267	0.0
79	1266	198.6	1277	0.6	1279	325.9	1278	0.3
80	1280	13.3	1296	0.0	1294	13.7	1292	14.2
81	1298	0.0	1305	21.3	1311	0.0	1324	0.0
82	1309	16.2	1307	10.2	1315	6.1	1339	26.6
83	1324	43.9	1335	0.0	1337	0.0	1344	399.3
84	1325	0.0	1343	0.0	1347	24.5	1348	0.0
85	1339	0.0	1350	0.9	1355	0.0	1351	0.0
86	1341	4.7	1366	0.0	1358	30.2	1369	105.3
87	1347	134.3	1369	2.4	1365	37.0	1372	7.7
88	1351	0.0	1373	0.0	1378	0.0	1385	0.0
89	1370	0.0	1378	0.0	1383	0.0	1413	0.0
90	1383	0.0	1393	0.0	1406	0.0	1422	0.0
91	1408	0.0	1429	0.0	1424	0.0	1425	0.0
92	1428	0.0	1435	4.6	1439	0.0	1441	0.0
93	1430	8.5	1438	0.0	1444	8.7	1449	2.3
94	1442	2.6	1448	15.4	1453	48.5	1453	100.4
95	1458	3.7	1481	6.6	1478	18.2	1472	197.6
96	1474	17.3	1483	0.0	1483	9.6	1486	61.8
97	1486	0.0	1492	2.3	1490	0.0	1494	0.0
98	1523	0.0	1531	0.0	1534	0.0	1518	0.0
99	1537	0.0	1537	0.0	1540	27.9	1527	19.5
100	1540	3.4	1552	0.6	1542	22.3	1543	0.0
101	1541	14.1	1565	0.0	1542	0.0	1546	190.7
102	1545	0.0	1565	0.7	1551	0.0	1551	0.0
103	1550	301.1	1588	13.6	1562	0.0	1564	0.0
104	1552	0.0	1597	0.0	1567	41.2	1568	232.4
105	1568	0.0	1598	0.0	1574	0.0	1568	128.2
106	1572	41.7	1603	38.9	1579	35.2	1576	0.0

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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})
107	3015	36.7	3046	14.8	3065	0.1	3068	0.8
108	3016	0.0	3046	0.0	3065	0.0	3068	0.0
109	3016	0.0	3050	0.0	3074	0.0	3083	0.0
110	3016	115.0	3050	6.7	3075	0.0	3083	0.2
111	3022	20.9	3051	1.4	3075	0.0	3083	1.5
112	3022	0.0	3052	0.0	3075	0.0	3084	0.0
113	3040	0.0	3066	0.0	3088	0.0	3096	0.8
114	3041	108.7	3067	140.1	3088	29.0	3096	0.0
115	3041	392.8	3070	48.4	3093	11.6	3103	1.1
116	3043	0.0	3070	0.0	3093	0.0	3103	0.0
117	3072	0.0	3083	0.0	3103	0.0	3110	0.0
118	3072	13.3	3083	24.0	3103	4.8	3110	0.7
119	3089	133.8	3097	86.8	3115	30.4	3120	0.2
120	3090	0.0	3097	0.0	3115	0.0	3120	0.0