

Harmonic vibrational frequencies of azulene ($C_{10}H_8$) 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	137	0.0	162	0.0	155	1.7	143	0.0
2	183	0.0	168	1.3	156	0.0	145	2.0
3	291	6.4	313	8.6	297	7.9	276	4.2
4	329	1.8	335	0.7	333	0.1	325	0.1
5	389	0.9	407	1.3	378	0.0	326	0.0
6	428	0.0	421	0.0	403	0.2	384	50.6
7	488	0.8	493	1.7	493	0.4	399	0.6
8	574	2.9	568	7.0	495	22.4	484	1.9
9	597	4.1	606	2.8	564	0.1	497	1.6
10	643	19.2	656	1.6	665	0.2	650	11.3
11	648	0.3	703	0.0	695	0.0	685	0.0
12	670	0.0	726	2.7	717	2.6	712	2.7
13	671	61.0	735	0.6	741	1.0	729	25.5
14	698	0.0	770	113.5	778	112.5	814	79.6
15	748	0.2	789	0.0	833	4.4	820	15.7
16	752	8.8	819	6.2	841	0.0	878	21.8
17	783	0.0	865	0.0	897	0.0	884	0.0
18	794	12.5	907	2.0	900	0.0	918	50.5
19	843	3.2	927	0.0	931	4.3	987	11.2
20	893	7.7	936	1.3	956	2.5	991	0.0
21	907	0.0	960	7.8	982	6.4	999	4.9
22	908	12.6	984	0.0	1024	0.0	1008	0.0
23	911	0.2	1003	0.0	1037	1.0	1048	0.0
24	1014	3.2	1015	13.5	1045	0.3	1057	4.1
25	1039	16.0	1045	1.0	1051	5.5	1066	1.6
26	1053	0.8	1060	4.8	1076	3.5	1085	21.1
27	1166	1.2	1166	0.6	1132	0.8	1093	15.7
28	1203	3.2	1224	5.7	1196	0.2	1130	112.4
29	1209	5.6	1226	2.9	1239	13.7	1239	0.1
30	1242	3.2	1268	1.7	1241	2.7	1260	24.3
31	1261	12.0	1304	0.1	1292	2.0	1300	0.1
32	1316	2.6	1320	2.7	1360	16.2	1353	3.1
33	1343	31.1	1386	90.3	1366	59.5	1388	212.6
34	1346	36.9	1402	0.0	1384	62.6	1394	4.1
35	1397	4.3	1451	7.7	1428	3.1	1457	35.5
36	1437	0.5	1467	6.6	1461	7.1	1471	16.5
37	1441	0.4	1488	10.8	1467	26.1	1511	1.9
38	1497	21.2	1542	5.9	1542	3.1	1526	59.2
39	1527	5.4	1590	55.8	1560	0.4	1573	8.1
40	1571	27.1	1598	2.0	1584	3.9	1583	4.5
41	2936	19.7	3009	0.1	3052	0.0	3057	1.3
42	2940	9.8	3011	16.8	3053	0.1	3058	1.8
43	2968	17.2	3019	10.4	3060	0.1	3065	0.9
44	2974	238.5	3040	48.2	3071	0.2	3068	38.6
45	2996	169.3	3050	38.6	3079	0.0	3076	28.8
46	3027	4.9	3092	6.6	3126	0.1	3100	3.8
47	3039	109.8	3108	17.6	3129	1.2	3101	51.3
48	3066	123.8	3121	23.8	3153	3.1	3145	64.5