Harmonic vibrational frequencies of terrylene ($C_{30}H_{16}$) 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	25	0.0	16	0.0	29	0.0	30	0.0
2	34	0.0	27	0.0	35	0.6	33	1.5
3	37	0.0	36	0.2	54	0.0	61	0.0
4	108	0.0	108	0.0	107	0.0	103	0.0
5	118	0.0	111	0.2	126	0.3	130	0.4
6	147	0.5	145	0.1	147	0.5	146	0.9
7	171	0.0	162	0.0	165	0.0	163	0.0
8	179	3.5	173	5.9	171	9.9	165	14.8
9	202	0.0	209	0.0	206	0.0	202	0.0
10	206	0.0	217	0.0	219	0.0	221	0.0
11	240	0.0	240	0.0	242	0.0	242	0.0
12	271	0.0	266	1.8	259	2.2	253	2.2
13	271	1.2	270	0.0	271	0.0	270	0.0
14	283	0.0	293	0.0	291	0.0	289	0.0
15	338	0.0	345	0.0	334	0.0	322	0.0
16	388	2.8	383	0.0	388	0.0	389	0.4
17	389	0.0	389	0.0	392	0.0	393	0.0
18	401	0.0	422	0.0	414	0.0	405	0.0
19	425	8.9	426	0.1	426	0.1	423	0.1
20	440	0.0	441	0.0	440	0.0	437	0.0
21	469	3.1	460	0.0	456	1.5	444	7.0
22	479	0.0	463	0.0	458	0.0	446	0.0
23	481	1.1	471	4.3	473	17.1	457	0.0
24	485	0.0	472	0.0	473	0.0	475	31.0
25	492	0.0	489	0.0	475	0.0	482	0.0
26	511	35.1	514	7.0	514	2.5	512	1.9
27	527	0.0	532	0.0	529	2.4	523	5.0
28	532	0.0	533	0.9	531	0.0	530	0.0
29	533	0.0	548	0.0	545	0.0	536	4.2
30	549	0.0	556	0.0	549	5.0	539	0.0
31	559	1.1	561	5.2	552	0.0	544	0.0
32	565	0.0	565	0.0	560	0.0	554	0.0
33	569	0.0	577	0.0	575	0.0	570	0.0
34	612	0.0	613	0.0	604	0.0	594	0.0
35	619	0.0	629	0.0	621	0.0	610	0.0
36	623	0.0	630	0.0	627	0.0	625	0.0
37	633	0.5	636	0.4	633	0.0	629	0.3
38	658	0.0	664	0.0	670	3.6	666	23.5
39	669	0.7	670	0.1	677	0.0	675	22.5
40	669	4.7	690	5.7	682	12.1	690	0.0
41	727	0.0	731	0.0	729	0.0	724	0.0
42	731	0.0	751	49.4	744	53.3	736	0.0
43	732	69.5	758	0.0	747	0.0	737	48.6
44	736	0.0	759	0.0	771	0.0	778	0.0
45	738	0.0	764	0.0	777	0.0	784	0.0
46	771	0.0	781	0.0	780	0.0	789	1.4
47	781	157.6	790	25.3	790	6.8	795	0.0
48	783	0.0	795	0.0	797	0.0	796	0.0
49	788	1.2	803	3.2	803	0.2	802	0.6
50	793	0.0	813	0.0	812	0.0	808	0.0
51	799	39.2	817	190.3	815	186.7	815	185.5
52	805	0.0	826	0.0	825	3.4	816	21.4

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Table 1 - continued from previous page

Numb. of the mode	Anion Freq. (cm^{-1})	Anion Int. (km mol^{-1})	Neutral Freq. (cm^{-1})	Neutral Int. (km mol^{-1})	Cation Freq. (cm^{-1})	Cation Int. (km mol^{-1})	Dication Freq. (cm^{-1})	Dication Int. (km mol^{-1})
53	814	0.0	831	2.6	832	0.0	838	0.0
54	816	0.0	835	0.0	836	0.0	841	0.0
55	820	9.9	841	0.0	843	0.2	848	0.9
56	824	0.2	882	0.0	909	0.0	926	42.3
57	826	0.0	883	0.0	909	0.0	938	0.0
58	840	0.0	902	0.0	921	5.0	939	0.0
59	842	6.5	903	0.4	930	0.0	954	0.0
60	902	0.0	914	15.1	931	3.3	961	0.0
61	908	0.0	941	0.0	958	0.0	962	5.6
62	913	33.6	946	0.0	969	0.0	989	0.0
63	934	0.0	960	0.0	972	0.0	990	0.0
64	936	0.0	971	0.0	993	0.0	1001	34.9
65	940	2.3	971	0.0	994	0.0	1015	0.0
66	942	0.0	979	2.5	1002	0.5	1016	0.0
67	954	0.0	980	0.0	1003	0.0	1025	0.0
68	1008	23.9	1021	2.0	1013	10.5	1025	0.0
69	1026	0.0	1026	0.0	1038	0.0	1041	0.0
70	1042	0.0	1051	0.0	1052	0.0	1045	0.0
71	1065	7.4	1062	2.1	1071	0.4	1072	0.0
72	1093	16.7	1095	2.7	1102	0.0	1104	19.4
73	1094	0.0	1096	0.0	1103	0.0	1105	0.0
74	1123	0.0	1139	0.0	1135	0.0	1125	0.0
75	1142	0.1	1153	2.9	1153	8.6	1145	18.1
76	1157	0.0	1164	0.0	1166	0.0	1150	0.0
77	1159	7.9	1165	0.0	1171	0.0	1173	8.7
78	1160	0.0	1175	0.0	1173	0.0	1178	0.0
79	1187	0.3	1199	0.0	1202	0.1	1203	0.7
80	1190	0.0	1199	0.0	1203	0.0	1208	0.0
81	1203	0.1	1212	7.7	1220	0.2	1226	2.2
82	1211	0.6	1212	3.8	1222	66.2	1231	173.4
83	1212	0.0	1215	0.0	1228	0.0	1232	0.0
84	1220	0.0	1224	0.0	1232	0.0	1238	46.0
85	1221	15.0	1234	2.0	1242	23.3	1239	0.0
86	1262	100.6	1267	1.2	1281	96.2	1281	1229.8
87	1274	0.0	1274	0.0	1284	0.0	1290	0.0
88	1276	477.8	1286	0.0	1290	492.0	1294	125.0
89	1287	0.0	1295	10.1	1305	0.0	1312	0.0
90	1292	0.0	1308	0.0	1306	0.0	1322	0.0
91	1307	49.0	1314	0.0	1318	3.2	1341	0.0
92	1323	0.0	1337	0.0	1343	0.0	1350	59.5
93	1331	0.0	1339	2.6	1349	0.0	1357	516.8
94	1331	138.4	1343	0.0	1351	104.0	1368	0.0
95	1338	0.3	1353	5.8	1360	0.5	1375	0.0
96	1351	0.0	1354	0.0	1365	0.0	1386	16.5
97	1366	22.7	1375	52.1	1383	75.0	1393	2.0
98	1391	2.4	1393	31.7	1403	7.9	1409	3.7
99	1406	0.0	1410	0.0	1420	0.0	1419	0.0
100	1415	0.0	1443	0.0	1437	0.0	1427	0.0
101	1436	15.4	1448	8.4	1448	0.0	1443	0.0
102	1439	0.0	1453	0.0	1451	0.0	1454	14.0
103	1442	0.0	1457	0.0	1458	28.6	1459	0.0
104	1449	3.9	1466	2.1	1460	2.9	1464	9.1
105	1485	11.0	1495	13.0	1488	4.8	1489	39.1
106	1498	0.0	1503	0.0	1502	0.0	1498	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	1527	70.1	1523	0.4	1536	33.0	1510	74.6
108	1536	0.6	1540	0.0	1539	2.9	1533	0.0
109	1540	0.0	1559	11.8	1541	434.7	1535	0.0
110	1541	465.5	1572	27.8	1548	0.0	1538	234.4
111	1541	0.0	1576	0.0	1550	0.0	1554	1.3
112	1558	0.0	1581	0.0	1557	0.0	1557	1271.9
113	1559	41.3	1582	30.8	1558	73.7	1564	0.0
114	1561	0.0	1583	0.0	1573	0.0	1567	0.0
115	1561	120.3	1599	10.4	1576	5.0	1575	41.0
116	1579	0.0	1601	0.0	1577	0.0	1589	0.0
117	3018	0.0	3049	0.0	3072	0.0	3080	0.2
118	3018	86.0	3049	8.5	3072	0.2	3080	0.0
119	3019	42.0	3051	2.2	3074	0.1	3083	0.0
120	3019	0.0	3051	0.0	3074	0.0	3083	1.5
121	3040	0.0	3066	0.0	3089	0.0	3099	1.4
122	3041	64.8	3067	28.8	3089	50.2	3099	0.0
123	3045	441.3	3068	206.0	3090	6.2	3101	0.8
124	3045	0.0	3069	0.0	3091	0.0	3101	0.0
125	3057	0.0	3075	0.0	3099	6.9	3108	1.8
126	3057	7.3	3076	12.2	3099	0.0	3108	0.0
127	3074	2.1	3086	15.2	3106	7.7	3113	0.0
128	3074	0.0	3086	0.0	3106	0.0	3113	0.0
129	3087	0.0	3096	0.0	3117	0.0	3125	0.0
130	3087	17.9	3096	19.0	3117	11.1	3125	0.6
131	3092	195.3	3103	95.9	3125	33.4	3133	3.6
132	3093	0.0	3104	0.0	3125	0.0	3134	0.0