

Supplementary information

Table 3: Frequencies, dipole strengths and rotational strengths of the four conformations of **1^a**

mode	I						II					III					IV				
	ν	D	R	49%D	49%R	ν	D	R	25%D	25%R	ν	D	R	15%D	15%R	ν	D	R	11%D	11%R	
123	3219	27.7	-5.7	13.6	-2.8	3220	9.1	-31.7	2.3	-7.9	3220	28.2	5.9	4.2	0.9	3221	23.5	5.4	2.6	0.6	
122	3219	33.6	15.5	16.6	7.6	3220	46.5	52.1	11.5	12.9	3220	28.3	7.4	4.2	1.1	3219	30.1	8.8	3.3	1.0	
121	3210	34.4	0.8	16.9	0.4	3210	56.2	-25.9	13.9	-6.4	3210	34.1	6.0	5.1	0.9	3211	31.8	-1.1	3.5	-0.1	
120	3209	26.1	1.4	12.9	0.7	3210	2.2	27.8	0.6	6.9	3210	32.0	-1.1	4.8	-0.2	3207	34.1	-3.1	3.8	-0.3	
119	3197	11.4	0.7	5.6	0.37	3199	4.2	18.0	1.0	4.5	3199	10.2	-1.0	1.5	-0.2	3200	10.1	-0.6	1.1	-0.1	
118	3197	10.6	-4.2	5.2	-2.1	3199	16.1	-27.8	4.0	-6.9	3199	10.8	-2.0	1.6	-0.3	3197	7.2	-3.3	0.8	-0.4	
117	3188	3.4	1.5	1.8	0.7	3188	1.7	6.3	0.4	1.6	3189	3.2	-1.5	0.5	-0.2	3190	3.8	-1.8	0.4	-0.2	
116	3188	2.1	-3.6	1.0	-1.8	3188	4.6	-13.5	1.1	-3.3	3189	2.7	-0.9	0.4	-0.1	3188	3.1	-2.0	0.3	-0.2	
115	3155	0.5	-2.3	0.3	-1.1	3162	0.6	2.8	0.2	0.7	3139	0.6	-2.1	0.1	-0.3	3140	0.8	2.6	0.1	0.3	
114	3113	112.4	125.7	55.4	61.9	3115	4.3	-15.5	1.1	-3.8	3117	51.9	18.9	7.8	2.8	3130	61.3	11.0	6.8	1.2	
113	3113	6.1	-67.0	3.0	-33.0	3115	108.3	60.5	26.8	15.0	3115	66.1	34.6	9.9	5.2	3114	57.1	42.7	6.3	4.7	
112	3104	4.6	-22.3	2.3	-11.0	3109	5.2	-44.2	1.3	-11.0	3109	9.8	-18.4	1.5	-2.8	3110	3.9	-5.0	0.4	-0.6	
111	3104	13.5	-14.8	6.7	-7.3	3109	32.0	-5.7	7.9	-1.4	3107	13.8	-23.3	2.1	-3.5	3108	22.8	-23.2	2.5	-2.6	
110	3100	0.2	-0.3	0.1	-0.2	3103	2.00	-0.5	0.5	-0.1	3082	3.6	-0.1	0.5	-0.0	3079	7.7	5.1	0.8	0.6	
109	3076	15.3	19.2	7.5	9.5	3076	15.2	-9.5	3.8	-2.4	3079	25.2	-13.9	3.8	-2.1	3077	22.6	-2.2	2.5	-0.2	
108	3076	34.7	-40.5	17.1	-20.0	3076	45.3	-14.7	11.2	-3.6	3077	24.6	-8.8	3.7	-1.3	3067	21.6	10.7	2.4	1.2	
107	3057	25.8	-5.7	12.7	-2.8	3060	16.9	35.3	4.2	8.7	3060	27.1	6.0	4.1	0.9	3062	40.7	-17.3	4.5	-1.9	
106	3057	25.6	14.6	12.6	7.2	3060	27.4	-26.5	6.8	-6.6	3059	25.4	3.3	3.8	0.5	3060	28.2	4.5	3.1	0.5	
105	1765	10.2	31.0	5.0	15.3	1763	2.7	-6.8	0.7	-1.7	1761	237.0	15.9	35.5	2.4	1760	316.5	13.3	34.9	1.5	
104	1747	842.6	38.6	414.9	19.0	1745	778.7	93.7	192.9	23.2	1758	475.8	32.9	71.2	4.9	1756	271.9	-47.7	30.0	-5.3	
103	1676	2.5	-14.6	1.2	-7.2	1676	0.1	-0.5	0.02	-0.1	1677	2.7	-14.4	0.4	-2.2	1677	1.9	-11.9	0.2	-1.3	
102	1675	2.4	-13.5	1.2	-6.7	1676	5.0	-31.5	1.2	-7.8	1676	1.9	-12.4	0.3	-1.9	1677	3.2	-13.5	0.4	-1.5	
101	1656	0.8	-2.3	0.4	-1.1	1656	0.2	-1.3	0.1	-0.3	1656	0.6	-1.8	0.1	-0.3	1658	0.8	-0.9	0.1	-0.1	
100	1656	0.8	-1.8	0.4	-0.9	1656	1.1	-1.9	0.3	-0.5	1655	0.9	-1.8	0.1	-0.3	1657	0.4	-2.0	0.0	-0.2	
99	1532	29.5	-8.1	14.5	-4.0	1533	15.7	-36.3	3.9	-9.0	1538	28.3	-6.0	4.2	-0.9	1534	31.6	-9.1	3.5	-1.0	
98	1532	29.9	-7.2	14.7	-3.5	1532	42.6	18.2	10.6	4.5	1532	29.7	-7.0	4.4	-1.1	1533	22.9	-4.4	2.5	-0.5	
97	1508	19.1	-10.6	9.4	-5.2	1509	18.7	15.4	4.6	3.8	1509	21.2	-15.6	3.2	-2.3	1510	20.0	-12.2	2.2	-1.4	
96	1508	19.8	-5.3	9.8	-2.6	1508	15.1	-33.9	3.7	-8.4	1508	20.2	-3.5	3.0	-0.5	1509	21.9	-10.4	2.4	-1.2	
95	1494	7.8	3.0	3.8	1.5	1495	6.1	10.6	1.5	2.6	1494	5.9	2.8	0.9	0.4	1495	12.2	4.7	1.4	0.5	
94	1493	7.8	3.0	3.8	1.5	1492	4.5	-1.9	1.1	-0.5	1493	8.8	3.8	1.3	0.6	1495	6.1	1.9	0.7	0.2	
93	1470	38.5	4.8	19.0	2.4	1472	34.7	8.4	8.6	2.1	1475	50.5	6.6	7.6	1.0	1475	46.5	1.4	5.1	0.2	
92	1406	102.6	15.0	50.5	7.4	1406	22.3	11.3	5.5	2.8	1436	191.6	73.2	28.7	11.0	1433	203.6	29.6	22.5	3.3	
91	1403	47.2	47.7	23.2	23.5	1402	115.2	-59.8	28.5	-14.8	1399	21.7	5.7	3.3	0.9	1396	4.6	-11.1	0.5	-1.2	
90	1391	5.7	3.0	2.8	1.5	1392	6.5	-13.3	1.6	-3.3	1392	10.2	-3.9	1.5	-0.6	1394	78.2	-11.2	8.6	-1.2	
89	1391	16.3	-11.3	8.0	-5.6	1392	10.6	6.5	2.6	1.6	1391	11.7	-4.2	1.8	-0.6	1392	2.6	-1.2	0.3	-0.1	
88	1360	20.9	2.7	10.3	1.3	1359	42.2	38.5	10.5	9.5	1372	19.5	7.3	2.9	1.1	1371	20.8	1.7	2.3	0.2	
87	1355	28.7	67.6	14.1	33.3	1356	3.9	-8.5	1.0	-2.1	1354	5.9	15.6	0.9	2.3	1351	26.4	29.7	2.9	3.3	
86	1346	28.9	13.4	14.2	6.6	1350	4.4	4.9	1.1	1.2	1349	4.9	-2.7	0.7	-0.4	1348	3.3	-2.1	0.4	-0.2	
85	1335	34.8	55.0	17.1	27.1	1337	52.6	-45.1	13.0	-11.2	1332	25.8	-16.7	3.9	-2.5	1334	24.7	5.5	2.7	0.6	
84	1326	5.5	-7.0	2.7	-3.5	1329	24.5	6.8	6.1	1.7	1328	17.6	-4.5	2.6	-0.7	1327	7.9	-9.6	0.9	-1.1	
83	1321	3.8	8.0	1.9	3.9	1321	74.3	-43.7	18.4	-10.8	1320	11.4	-6.2	1.7	-0.9	1324	24.2	-23.1	2.7	-2.6	
82	1318	0.7	0.9	0.3	0.4	1318	7.3	-2.3	1.8	-0.6	1319	19.2	-5.2	2.9	-0.8	1318	1.5	0.2	0.2	0.0	
81	1318	11.9	-6.3	5.9	-3.1	1318	6.3	2.3	1.6	0.6	1317	36.0	-18.3	5.4	-2.7	1311	23.5	11.2	2.6	1.2	
80	1302	286.5	-96.3	141.1	-47.4	1294	66.4	-6.6	16.5	-1.6	1296	113.9	-29.0	17.1	-4.3	1296	48.0	-34.8	5.3	-3.8	
79	1281	57.2	100.7	28.2	49.6	1280	6.1	-4.9	1.5	-1.2	1276	45.7	12.4	6.8	1.9	1275	80.4	27.4	8.9	3.0	
78	1258	163.8	-72.4	80.7	-35.7	1258	184.8	79.3	45.8	19.6	1252	3.0	2.5	0.5	0.4	1252	1.3	-1.1	0.1	-0.1	
77	1251	0.1	0.7	0.1	0.4	1251	1.8	0.9	0.5	0.2	1251	2.3	-6.0	0.3	-0.9	1249	4.2	2.2	0.5	0.2	
76	1250	10.4	-7.7	5.1	-3.8	1250	13.2	17.4	3.3	4.3	1239	23.9	11.9	3.6	1.8	1239	6.5	-2.8	0.7	-0.3	