

Supporting information

Bellow are given the fundamental vibrational frequencies of the spherophanes studied in the paper :

Theoretical Study of Spherophanes' Geometrical and Electronic Structures

Saal A.,^{a,c} Daul C.A.,^a Jarrosson T.,^b Ouamerali O.^c

^a Department of Chemistry University of Fribourg, Switzerland;

^b Ecole ENSCM, Montpellier, France;

^c LPCTCI Laboratory, Faculty of Chemistry, USTHB University of Algiers, Algeria.

Table A: Fundamental normal modes vibrational frequency, their scaled values (by the factor 0.9613) as well as their symmetry obtained at B3LYP/6-31G(d) of the four octahedral spherophanes considered. The frequencies in blue are Raman active and the red ones are infra-red active.

Spher1 (Oh)															
N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm
1	85.2	81.9	EU	54	604.0	580.6	T1G	107	989.4	951.1	A2U	159	1427.2	1371.9	T1G
2	85.2	81.9	EU	55	604.0	580.6	T1G	108	999.2	960.5	T2G	160	1427.8	1372.6	A2G
3	143.7	138.2	T2G	56	609.3	585.7	T1U	109	999.2	960.5	T2G	161	1433.2	1377.7	EG
4	143.7	138.2	T2G	57	609.3	585.7	T1U	110	999.2	960.5	T2G	162	1433.2	1377.7	EG
5	143.7	138.2	T2G	58	609.3	585.7	T1U	111	1017.6	978.2	A2U	163	1475.4	1418.3	EU
6	185.4	178.3	A2U	59	628.7	604.4	A2U	112	1019.3	979.9	T1U	164	1475.4	1418.3	EU
7	188.9	181.5	EG	60	664.9	639.1	EU	113	1019.3	979.9	T1U	165	1505.6	1447.3	T2U
8	188.9	181.5	EG	61	664.9	639.1	EU	114	1019.3	979.9	T1U	166	1505.6	1447.3	T2U
9	206.9	198.9	T2U	62	670.5	644.6	T2G	115	1041.8	1001.5	A1G	167	1505.6	1447.3	T2U
10	206.9	198.9	T2U	63	670.5	644.6	T2G	116	1112.0	1069.0	EU	168	1511.8	1453.3	T2G
11	206.9	198.9	T2U	64	670.5	644.6	T2G	117	1112.0	1069.0	EU	169	1511.8	1453.3	T2G
12	231.2	222.2	T2G	65	676.7	650.5	T1G	118	1117.7	1074.4	T2G	170	1511.8	1453.3	T2G
13	231.2	222.2	T2G	66	676.7	650.5	T1G	119	1117.7	1074.4	T2G	171	1592.6	1531.0	T2U
14	231.2	222.2	T2G	67	676.7	650.5	T1G	120	1117.7	1074.4	T2G	172	1592.6	1531.0	T2U
15	295.6	284.1	T1G	68	678.7	652.4	T1U	121	1124.8	1081.2	T1G	173	1592.6	1531.0	T2U
16	295.6	284.1	T1G	69	678.7	652.4	T1U	122	1124.8	1081.2	T1G	174	1595.5	1533.8	EG
17	295.6	284.1	T1G	70	678.7	652.4	T1U	123	1124.8	1081.2	T1G	175	1595.5	1533.8	EG
18	304.7	293.0	T1U	71	721.2	693.3	A1G	124	1155.7	1110.9	T1U	176	1599.0	1537.1	T1G
19	304.7	293.0	T1U	72	740.9	712.3	T1U	125	1155.7	1110.9	T1U	177	1599.0	1537.1	T1G
20	304.7	293.0	T1U	73	740.9	712.3	T1U	126	1155.7	1110.9	T1U	178	1599.0	1537.1	T1G
21	306.8	294.9	EU	74	740.9	712.3	T1U	127	1188.0	1142.1	T2G	179	1600.1	1538.1	T1U
22	306.8	294.9	EU	75	775.1	745.2	T2G	128	1188.0	1142.1	T2G	180	1600.1	1538.1	T1U
23	350.9	337.3	A2G	76	775.1	745.2	T2G	129	1188.0	1142.1	T2G	181	1600.1	1538.1	T1U
24	362.4	348.4	T2U	77	775.1	745.2	T2G	130	1190.2	1144.1	T2U	182	1600.9	1538.9	T2G
25	362.4	348.4	T2U	78	831.5	799.3	A2U	131	1190.2	1144.1	T2U	183	1600.9	1538.9	T2G
26	362.4	348.4	T2U	79	845.2	812.5	T2G	132	1190.2	1144.1	T2U	184	1600.9	1538.9	T2G
27	376.1	361.6	A1G	80	845.2	812.5	T2G	133	1207.2	1160.5	A1U	185	1608.2	1546.0	EU
28	428.6	412.0	T1U	81	845.2	812.5	T2G	134	1215.6	1168.6	T1U	186	1608.2	1546.0	EU
29	428.6	412.0	T1U	82	846.0	813.3	EU	135	1215.6	1168.6	T1U	187	3251.8	3126.0	EU
30	428.6	412.0	T1U	83	846.0	813.3	EU	136	1215.6	1168.6	T1U	188	3251.8	3126.0	EU
31	431.3	414.6	T2G	84	869.4	835.7	T2G	137	1216.3	1169.2	EG	189	3252.3	3126.4	T2G
32	431.3	414.6	T2G	85	869.4	835.7	T2G	138	1216.3	1169.2	EG	190	3252.3	3126.4	T2G
33	431.3	414.6	T2G	86	869.4	835.7	T2G	139	1246.4	1198.1	A1G	191	3252.3	3126.4	T2G
34	488.6	469.7	EG	87	881.8	847.7	T1U	140	1251.7	1203.3	T1G	192	3253.0	3127.1	A2U
35	488.6	469.7	EG	88	881.8	847.7	T1U	141	1251.7	1203.3	T1G	193	3277.9	3151.1	T1G
36	491.7	472.7	T2U	89	881.8	847.7	T1U	142	1251.7	1203.3	T1G	194	3277.9	3151.1	T1G
37	491.7	472.7	T2U	90	886.5	852.2	T2U	143	1293.4	1243.3	T2U	195	3277.9	3151.1	T1G
38	491.7	472.7	T2U	91	886.5	852.2	T2U	144	1293.4	1243.3	T2U	196	3278.9	3152.0	T1U
39	531.9	511.4	EG	92	886.5	852.2	T2U	145	1293.4	1243.3	T2U	197	3278.9	3152.0	T1U
40	531.9	511.4	EG	93	904.2	869.2	EG	146	1314.5	1263.6	A1U	198	3278.9	3152.0	T1U
41	534.8	514.1	T1G	94	904.2	869.2	EG	147	1321.4	1270.3	A2G	199	3279.0	3152.1	T2U
42	534.8	514.1	T1G	95	907.2	872.1	T1G	148	1356.9	1304.4	T1G	200	3279.0	3152.1	T2U
43	534.8	514.1	T1G	96	907.2	872.1	T1G	149	1356.9	1304.4	T1G	201	3279.0	3152.1	T2U
44	544.9	523.8	T2G	97	907.2	872.1	T1G	150	1356.9	1304.4	T1G	202	3279.7	3152.7	T2G
45	544.9	523.8	T2G	98	911.7	876.4	T2U	151	1393.3	1339.4	T2U	203	3279.7	3152.7	T2G
46	544.9	523.8	T2G	99	911.7	876.4	T2U	152	1393.3	1339.4	T2U	204	3279.7	3152.7	T2G
47	547.6	526.4	T2U	100	911.7	876.4	T2U	153	1393.3	1339.4	T2U	205	3307.6	3179.6	T1U
48	547.6	526.4	T2U	101	931.3	895.3	A1G	154	1403.7	1349.3	T1U	206	3307.6	3179.6	T1U
49	547.6	526.4	T2U	102	953.2	916.3	T1U	155	1403.7	1349.3	T1U	207	3307.6	3179.6	T1U
50	560.5	538.8	EU	103	953.2	916.3	T1U	156	1403.7	1349.3	T1U	208	3307.6	3179.6	EG
51	560.5	538.8	EU	104	953.2	916.3	T1U	157	1427.2	1371.9	T1G	209	3307.6	3179.6	EG
52	573.9	551.7	A1U	105	965.1	927.7	EG	158	1427.2	1371.9	T1G	210	3308.0	3180.0	A1G

53	604.0	580.6	T1G	106	965.1	927.7	EG
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Meth2 (Oh)

N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm
1	57.0	54.8	A2G	81	594.1	571.1	T2G	161	1018.1	978.7	T1U	241	1508.5	1450.1	T2G
2	61.6	59.2	T2U	82	602.3	579.0	A1G	162	1019.6	980.1	A1G	242	1508.5	1450.1	T2G
3	61.6	59.2	T2U	83	650.4	625.3	A2U	163	1175.4	1129.9	A1U	243	1515.7	1457.0	A1G
4	61.6	59.2	T2U	84	660.8	635.2	T1U	164	1181.2	1135.5	T1G	244	1516.0	1457.3	T1U
5	65.4	62.8	EG	85	660.8	635.2	T1U	165	1181.2	1135.5	T1G	245	1516.0	1457.3	T1U
6	65.4	62.8	EG	86	660.8	635.2	T1U	166	1181.2	1135.5	T1G	246	1516.0	1457.3	T1U
7	91.9	88.4	T2G	87	683.4	656.9	T2G	167	1181.5	1135.7	T2U	247	1517.0	1458.3	EG
8	91.9	88.4	T2G	88	683.4	656.9	T2G	168	1181.5	1135.7	T2U	248	1517.0	1458.3	EG
9	91.9	88.4	T2G	89	683.4	656.9	T2G	169	1181.5	1135.7	T2U	249	1518.2	1459.5	T2G
10	111.9	107.6	A2U	90	704.1	676.9	A2U	170	1182.9	1137.1	T2G	250	1518.2	1459.5	T2G
11	127.2	122.3	EU	91	727.7	699.6	T2U	171	1182.9	1137.1	T2G	251	1518.2	1459.5	T2G
12	127.2	122.3	EU	92	727.7	699.6	T2U	172	1182.9	1137.1	T2G	252	1518.3	1459.5	T2U
13	165.3	158.9	T2G	93	727.7	699.6	T2U	173	1186.3	1140.4	EU	253	1518.3	1459.5	T2U
14	165.3	158.9	T2G	94	731.3	703.0	EG	174	1186.3	1140.4	EU	254	1518.3	1459.5	T2U
15	165.3	158.9	T2G	95	731.3	703.0	EG	175	1197.5	1151.1	T1G	255	1648.2	1584.4	T1G
16	186.4	179.2	T1U	96	754.9	725.7	T2G	176	1197.5	1151.1	T1G	256	1648.2	1584.4	T1G
17	186.4	179.2	T1U	97	754.9	725.7	T2G	177	1197.5	1151.1	T1G	257	1648.2	1584.4	T1G
18	186.4	179.2	T1U	98	754.9	725.7	T2G	178	1198.2	1151.8	T1U	258	1649.2	1585.4	EU
19	187.7	180.5	T2U	99	760.4	731.0	T1U	179	1198.2	1151.8	T1U	259	1649.2	1585.4	EU
20	187.7	180.5	T2U	100	760.4	731.0	T1U	180	1198.2	1151.8	T1U	260	1653.8	1589.8	T1U
21	187.7	180.5	T2U	101	760.4	731.0	T1U	181	1198.8	1152.4	EG	261	1653.8	1589.8	T1U
22	198.8	191.1	EU	102	765.0	735.4	A1G	182	1198.8	1152.4	EG	262	1653.8	1589.8	T1U
23	198.8	191.1	EU	103	863.5	830.1	A2U	183	1203.1	1156.5	T2U	263	1658.9	1594.7	T2G
24	201.5	193.7	T1G	104	873.6	839.8	T2G	184	1203.1	1156.5	T2U	264	1658.9	1594.7	T2G
25	201.5	193.7	T1G	105	873.6	839.8	T2G	185	1203.1	1156.5	T2U	265	1658.9	1594.7	T2G
26	201.5	193.7	T1G	106	873.6	839.8	T2G	186	1204.5	1157.9	EU	266	1661.0	1596.7	EG
27	210.9	202.7	A1G	107	886.7	852.3	EU	187	1204.5	1157.9	EU	267	1661.0	1596.7	EG
28	239.3	230.0	T1U	108	886.7	852.3	EU	188	1207.6	1160.8	T2G	268	1661.7	1597.4	T2U
29	239.3	230.0	T1U	109	887.6	853.3	EG	189	1207.6	1160.8	T2G	269	1661.7	1597.4	T2U
30	239.3	230.0	T1U	110	887.6	853.3	EG	190	1207.6	1160.8	T2G	270	1661.7	1597.4	T2U
31	263.7	253.5	T2G	111	891.6	857.1	T1U	191	1297.0	1246.8	A2U	271	3050.8	2932.8	T2U
32	263.7	253.5	T2G	112	891.6	857.1	T1U	192	1299.3	1249.0	T2G	272	3050.8	2932.8	T2U
33	263.7	253.5	T2G	113	891.6	857.1	T1U	193	1299.3	1249.0	T2G	273	3050.8	2932.8	T2U
34	268.6	258.2	EG	114	896.4	861.7	T1G	194	1299.3	1249.0	T2G	274	3050.9	2932.8	EG
35	268.6	258.2	EG	115	896.4	861.7	T1G	195	1302.9	1252.5	T1U	275	3050.9	2932.8	EG
36	270.8	260.3	T1G	116	896.4	861.7	T1G	196	1302.9	1252.5	T1U	276	3051.0	2932.9	T2G
37	270.8	260.3	T1G	117	896.4	861.7	T2U	197	1302.9	1252.5	T1U	277	3051.0	2932.9	T2G
38	270.8	260.3	T1G	118	896.4	861.7	T2U	198	1308.8	1258.2	A1G	278	3051.0	2932.9	T2G
39	279.1	268.3	T2U	119	896.4	861.7	T2U	199	1329.7	1278.2	A2G	279	3051.3	2933.2	T1U
40	279.1	268.3	T2U	120	900.1	865.3	T1U	200	1338.5	1286.7	T2U	280	3051.3	2933.2	T1U
41	279.1	268.3	T2U	121	900.1	865.3	T1U	201	1338.5	1286.7	T2U	281	3051.3	2933.2	T1U
42	335.2	322.2	T1U	122	900.1	865.3	T1U	202	1338.5	1286.7	T2U	282	3051.9	2933.8	A1G
43	335.2	322.2	T1U	123	902.5	867.6	T2G	203	1343.2	1291.2	T1G	283	3091.6	2972.0	A2G
44	335.2	322.2	T1U	124	902.5	867.6	T2G	204	1343.2	1291.2	T1G	284	3091.9	2972.2	T2U
45	335.6	322.6	EG	125	902.5	867.6	T2G	205	1343.2	1291.2	T1G	285	3091.9	2972.2	T2U
46	335.6	322.6	EG	126	926.3	890.5	EG	206	1343.2	1291.2	EU	286	3091.9	2972.2	T2U
47	422.4	406.0	A1U	127	926.3	890.5	EG	207	1343.2	1291.2	EU	287	3092.1	2972.4	T1G
48	445.0	427.8	T1G	128	926.6	890.7	T1G	208	1343.4	1291.4	T1G	288	3092.1	2972.4	T1G
49	445.0	427.8	T1G	129	926.6	890.7	T1G	209	1343.4	1291.4	T1G	289	3092.1	2972.4	T1G
50	445.0	427.8	T1G	130	926.6	890.7	T1G	210	1343.4	1291.4	T1G	290	3092.4	2972.7	T1U
51	456.3	438.7	T2U	131	927.3	891.4	T1U	211	1343.5	1291.5	A1U	291	3092.4	2972.7	T1U
52	456.3	438.7	T2U	132	927.3	891.4	T1U	212	1348.2	1296.0	T1U	292	3092.4	2972.7	T1U
53	456.3	438.7	T2U	133	927.3	891.4	T1U	213	1348.2	1296.0	T1U	293	3092.4	2972.7	EG
54	465.8	447.7	A2G	134	929.2	893.2	A1G	214	1348.2	1296.0	T1U	294	3092.4	2972.7	EG
55	479.6	461.0	EG	135	940.4	904.0	T2U	215	1351.2	1298.9	T2G	295	3165.1	3042.6	EU
56	479.6	461.0	EG	136	940.4	904.0	T2U	216	1351.2	1298.9	T2G	296	3165.1	3042.6	EU
57	481.2	462.6	T2U	137	940.4	904.0	T2U	217	1351.2	1298.9	T2G	297	3165.8	3043.3	T2G
58	481.2	462.6	T2U	138	967.9	930.4	T2G	218	1353.5	1301.1	A2U	298	3165.8	3043.3	T2G
59	481.2	462.6	T2U	139	967.9	930.4	T2G	219	1362.0	1309.3	T2U	299	3165.8	3043.3	T2G
60	487.3	468.4	T2G	140	967.9	930.4	T2G	220	1362.0	1309.3	T2U	300	3168.1	3045.5	T1G
61	487.3	468.4	T2G	141	986.2	948.0	A2G	221	1362.0	1309.3	T2U	301	3168.1	3045.5	T1G
62	487.3	468.4	T2G	142	987.8	949.5	EU	222	1362.2	1309.5	A2G	302	3168.1	3045.5	T1G
63	506.2	486.6	T1U	143	987.8	949.5	EU	223	1365.3	1312.5	T1G	303	3168.2	3045.5	T2U
64	506.2	486.6	T1U	144	989.0	950.7	T2U	224	1365.3	1312.5	T1G	304	3168.2	3045.5	T2U
65	506.2	486.6	T1U	145	989.0	950.7	T2U	225	1365.3	1312.5	T1G	305	3168.2	3045.5	T2U
66	524.5	504.2	EU	146	989.0	950.7	T2U	226	1372.9	1319.8	A1U	306	3168.5	3045.9	A2U
67	524.5	504.2	EU	147	991.9	953.5	EG	227	1496.3	1438.4	T1U	307	3169.9	3047.2	T1U
68	528.6	508.1	T1G	148	991.9	953.5	EG	228	1496.3	1438.4	T1U	308	3169.9	3047.2	T1U
69	528.6	508.1	T1G	149	1011.5	972.3	T1U	229	1496.3	1438.4	T1U	309	3169.9	3047.2	T1U
70	528.6	508.1	T1G	150	1011.5	972.3	T1U	230	1497.2	1439.2	EG	310	3170.5	3047.8	T2G
71	564.8	542.9	T1U	151	1011.5	972.3	T1U	231	1497.2	1439.2	EG	311	3170.5	3047.8	T2G
72	564.8	542.9	T1U	152	1014.5	975.2	A2U	232	1500.1	1442.1	T1G	312	3170.5	3047.8	T2G
73	564.8	542.9	T1U	153	1015.8	976.5	T2G	233	1500.1	1442.1	T1G	313	3172.3	3049.6	EG
74	567.2	545.3	EU	154	1015.8	976.5	T2G	234	1500.1	1442.1	T1G	314	3172.3	3049.6	EG
75	567.2	545.3	EU	155	1015.8	976.5	T2G	235	1505.4	1447.1	T2U	315	3173.2	3050.4	T1U
76	569.3	547.3	T1G	156	1017.1	977.7	T1G	236	1505.4	1447.1	T2U	316	3173.2	3050.4	T1U
77	569.3	547.3	T1G	157	1017.1	977.7	T1G	237	1505.4	1447.1	T2U	317	3173.2	3050.4	T1U
78	569.3	547.3	T1G	158	1017.1	977.7	T1G	238	1508.4	1450.0	EU	318	3174.0	3051.2	A1G
79	594.1	571.1	T2G	159	1018.1	978.7	T1U	239	1508.4	1450.0	EU				
80	594.1	571.1	T2G	160	1018.1	978.7	T1U	240	1508.5	1450.1	T2G				

Oxal 3 (Oh)

N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm
1	61.8	59.4	T2U	63	536.9	516.2	EU	125	904.8	869.8	T1U	187	1345.5	1293.5	T2U
2	61.8	59.4	T2U	64	549.7	528.5	T1G	126	910.3	875.1	A1G	188	1345.5	1293.5	T2U
3	61.8	59.4	T2U	65	549.7	528.5	T1G	127	962.8	925.5	T2U	189	1345.5	1293.5	T2U
4	62.2	59.8	A2G	66	549.7	528.5	T1G	128	962.8	925.5	T2U	190	1348.9	1296.7	A2G
5	70.0	67.3	EG	67	552.7	531.3	A1G	129	962.8	925.5	T2U	191	1469.5	1412.6	T1G
6	70.0	67.3	EG	68	565.7	543.8	T2U	130	966.9	929.5	EG	192	1469.5	1412.6	T1G

7	108.9	104.7	T2G	69	565.7	543.8	T2U	131	966.9	929.5	EG	193	1469.5	1412.6	T1G
8	108.9	104.7	T2G	70	565.7	543.8	T2U	132	998.8	960.2	T2G	194	1469.6	1412.7	EU
9	108.9	104.7	T2G	71	578.0	555.6	T1U	133	998.8	960.2	T2G	195	1469.6	1412.7	EU
10	127.7	122.8	A2U	72	578.0	555.6	T1U	134	998.8	960.2	T2G	196	1483.4	1426.0	T1U
11	144.2	138.7	EU	73	578.0	555.6	T1U	135	1019.8	980.3	A2U	197	1483.4	1426.0	T1U
12	144.2	138.7	EU	74	587.8	565.1	A2G	136	1021.7	982.2	T1U	198	1483.4	1426.0	T1U
13	184.6	177.5	T2G	75	599.2	576.0	EU	137	1021.7	982.2	T1U	199	1488.8	1431.2	EG
14	184.6	177.5	T2G	76	599.2	576.0	EU	138	1021.7	982.2	T1U	200	1488.8	1431.2	EG
15	184.6	177.5	T2G	77	602.9	579.6	T1G	139	1022.6	983.1	T2G	201	1489.3	1431.7	T2G
16	204.9	197.0	T1U	78	602.9	579.6	T1G	140	1022.6	983.1	T2G	202	1489.3	1431.7	T2G
17	204.9	197.0	T1U	79	602.9	579.6	T1G	141	1022.6	983.1	T2G	203	1489.3	1431.7	T2G
18	204.9	197.0	T1U	80	617.0	593.1	T2G	142	1027.2	987.5	EU	204	1490.1	1432.5	T2U
19	216.3	207.9	T1G	81	617.0	593.1	T2G	143	1027.2	987.5	EU	205	1490.1	1432.5	T2U
20	216.3	207.9	T1G	82	617.0	593.1	T2G	144	1029.4	989.5	A1G	206	1490.1	1432.5	T2U
21	216.3	207.9	T1G	83	658.0	632.5	T1U	145	1031.0	991.1	T1G	207	1621.8	1559.0	T1G
22	218.7	210.2	T2U	84	658.0	632.5	T1U	146	1031.0	991.1	T1G	208	1621.8	1559.0	T1G
23	218.7	210.2	T2U	85	658.0	632.5	T1U	147	1031.0	991.1	T1G	209	1621.8	1559.0	T1G
24	218.7	210.2	T2U	86	673.5	647.4	A2U	148	1032.0	992.1	T1U	210	1623.4	1560.5	EU
25	221.3	212.7	EU	87	673.5	647.5	T2G	149	1032.0	992.1	T1U	211	1623.4	1560.5	EU
26	221.3	212.7	EU	88	673.5	647.5	T2G	150	1032.0	992.1	T1U	212	1641.4	1577.8	T1U
27	239.1	229.8	A1G	89	673.5	647.5	T2G	151	1134.1	1090.2	T2U	213	1641.4	1577.8	T1U
28	268.5	258.1	T1U	90	698.1	671.1	A2U	152	1134.1	1090.2	T2U	214	1641.4	1577.8	T1U
29	268.5	258.1	T1U	91	732.3	703.9	T2U	153	1134.1	1090.2	T2U	215	1652.1	1588.2	T2G
30	268.5	258.1	T1U	92	732.3	703.9	T2U	154	1138.4	1094.3	EG	216	1652.1	1588.2	T2G
31	288.5	277.3	T2G	93	732.3	703.9	T2U	155	1138.4	1094.3	EG	217	1652.1	1588.2	T2G
32	288.5	277.3	T2G	94	733.8	705.4	T1U	156	1139.7	1095.6	T2G	218	1658.0	1593.8	EG
33	288.5	277.3	T2G	95	733.8	705.4	T1U	157	1139.7	1095.6	T2G	219	1658.0	1593.8	EG
34	298.1	286.6	EG	96	733.8	705.4	T1U	158	1139.7	1095.6	T2G	220	1658.9	1594.7	T2U
35	298.1	286.6	EG	97	735.3	706.9	T2G	159	1144.6	1100.3	EU	221	1658.9	1594.7	T2U
36	301.7	290.1	T2U	98	735.3	706.9	T2G	160	1144.6	1100.3	EU	222	1658.9	1594.7	T2U
37	301.7	290.1	T2U	99	735.3	706.9	T2G	161	1146.6	1102.3	T1G	223	3236.7	3111.4	EU
38	301.7	290.1	T2U	100	736.0	707.6	A1G	162	1146.6	1102.3	T1G	224	3236.7	3111.4	EU
39	316.2	304.0	T1G	101	739.7	711.1	EG	163	1146.6	1102.3	T1G	225	3236.8	3111.5	T2G
40	316.2	304.0	T1G	102	739.7	711.1	EG	164	1154.4	1109.7	T1U	226	3236.8	3111.5	T2G
41	316.2	304.0	T1G	103	845.4	812.7	A2U	165	1154.4	1109.7	T1U	227	3236.8	3111.5	T2G
42	394.3	379.0	EG	104	847.6	814.8	T2G	166	1154.4	1109.7	T1U	228	3236.9	3111.7	A2U
43	394.3	379.0	EG	105	847.6	814.8	T2G	167	1239.2	1191.2	A1U	229	3241.3	3115.8	T1U
44	397.6	382.2	T1U	106	847.6	814.8	T2G	168	1247.3	1199.1	T1G	230	3241.3	3115.8	T1U
45	397.6	382.2	T1U	107	850.8	817.9	EU	169	1247.3	1199.1	T1G	231	3241.3	3115.8	T1U
46	397.6	382.2	T1U	108	850.8	817.9	EU	170	1247.3	1199.1	T1G	232	3241.3	3115.8	T2G
47	472.8	454.5	EG	109	864.1	830.7	T1G	171	1254.7	1206.1	T2U	233	3241.3	3115.8	T2G
48	472.8	454.5	EG	110	864.1	830.7	T1G	172	1254.7	1206.1	T2U	234	3241.3	3115.8	T2G
49	473.0	454.7	T2U	111	864.1	830.7	T1G	173	1254.7	1206.1	T2U	235	3241.3	3115.9	T1G
50	473.0	454.7	T2U	112	864.7	831.3	T1U	174	1261.2	1212.4	A2G	236	3241.3	3115.9	T1G
51	473.0	454.7	T2U	113	864.7	831.3	T1U	175	1320.9	1269.8	T1U	237	3241.3	3115.9	T1G
52	481.4	462.7	T2G	114	864.7	831.3	T1U	176	1320.9	1269.8	T1U	238	3241.4	3116.0	T2U
53	481.4	462.7	T2G	115	883.7	849.5	T2U	177	1320.9	1269.8	T1U	239	3241.4	3116.0	T2U
54	481.4	462.7	T2G	116	883.7	849.5	T2U	178	1321.3	1270.2	A1G	240	3241.4	3116.0	T2U
55	483.1	464.4	A1U	117	883.7	849.5	T2U	179	1327.5	1276.1	T2G	241	3246.3	3120.7	A1G
56	500.5	481.2	T1U	118	888.6	854.2	T2G	180	1327.5	1276.1	T2G	242	3246.8	3121.1	T1U
57	500.5	481.2	T1U	119	888.6	854.2	T2G	181	1327.5	1276.1	T2G	243	3246.8	3121.1	T1U
58	500.5	481.2	T1U	120	888.6	854.2	T2G	182	1336.7	1285.0	A2U	244	3246.8	3121.1	T1U
59	527.4	507.0	T1G	121	896.9	862.2	EG	183	1338.4	1286.6	A1U	245	3247.0	3121.3	EG
60	527.4	507.0	T1G	122	896.9	862.2	EG	184	1342.0	1290.1	T1G	246	3247.0	3121.3	EG
61	527.4	507.0	T1G	123	904.8	869.8	T1U	185	1342.0	1290.1	T1G				
62	536.9	516.2	EU	124	904.8	869.8	T1U	186	1342.0	1290.1	T1G				

Thia4 (Oh)

N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm	N	freq	Scal. Freq	Symm
1	28.8	27.7	A2G	63	417.2	401.1	T1G	125	906.2	871.1	T1U	187	1325.7	1274.4	T2U
2	40.2	38.6	T2U	64	427.1	410.6	T2U	126	916.4	880.9	A1G	188	1325.7	1274.4	T2U
3	40.2	38.6	T2U	65	427.1	410.6	T2U	127	923.2	887.4	EU	189	1325.7	1274.4	T2U
4	40.2	38.6	T2U	66	427.1	410.6	T2U	128	923.2	887.4	EU	190	1327.9	1276.5	A2G
5	46.2	44.4	EG	67	428.2	411.6	T2G	129	928.2	892.3	T2G	191	1430.7	1375.3	T1G
6	46.2	44.4	EG	68	428.2	411.6	T2G	130	928.2	892.3	T2G	192	1430.7	1375.3	T1G
7	74.6	71.7	T2G	69	428.2	411.6	T2G	131	928.2	892.3	T2G	193	1430.7	1375.3	T1G
8	74.6	71.7	T2G	70	433.9	417.1	T1U	132	929.3	893.3	T1G	194	1432.0	1376.6	T1U
9	74.6	71.7	T2G	71	433.9	417.1	T1U	133	929.3	893.3	T1G	195	1432.0	1376.6	T1U
10	94.9	91.2	A2U	72	433.9	417.1	T1U	134	929.3	893.3	T1G	196	1432.0	1376.6	T1U
11	105.2	101.2	EU	73	434.3	417.5	A2G	135	932.3	896.2	T2U	197	1433.3	1377.8	EU
12	105.2	101.2	EU	74	436.9	420.0	EU	136	932.3	896.2	T2U	198	1433.3	1377.8	EU
13	135.2	130.0	T2U	75	436.9	420.0	EU	137	932.3	896.2	T2U	199	1435.2	1379.6	EG
14	135.2	130.0	T2U	76	437.1	420.2	T1G	138	937.4	901.1	T1U	200	1435.2	1379.6	EG
15	135.2	130.0	T2U	77	437.1	420.2	T1G	139	937.4	901.1	T1U	201	1437.6	1382.0	T2G
16	140.9	135.4	T2G	78	437.1	420.2	T1G	140	937.4	901.1	T1U	202	1437.6	1382.0	T2G
17	140.9	135.4	T2G	79	514.7	494.8	EU	141	940.9	904.5	EG	203	1437.6	1382.0	T2G
18	140.9	135.4	T2G	80	514.7	494.8	EU	142	940.9	904.5	EG	204	1437.8	1382.1	T2U
19	158.4	152.2	T1U	81	517.1	497.0	T1G	143	1006.5	967.5	A2U	205	1437.8	1382.1	T2U
20	158.4	152.2	T1U	82	517.1	497.0	T1G	144	1008.4	969.3	T2G	206	1437.8	1382.1	T2U
21	158.4	152.2	T1U	83	517.1	497.0	T1G	145	1008.4	969.3	T2G	207	1593.3	1531.6	T1G
22	170.4	163.8	A1G	84	558.6	537.0	T1U	146	1008.4	969.3	T2G	208	1593.3	1531.6	T1G
23	184.8	177.7	EU	85	558.6	537.0	T1U	147	1010.9	971.7	T1U	209	1593.3	1531.6	T1G
24	184.8	177.7	EU	86	558.6	537.0	T1U	148	1010.9	971.7	T1U	210	1593.6	1531.9	EU
25	185.3	178.1	T1G	87	587.4	564.7	T2G	149	1010.9	971.7	T1U	211	1593.6	1531.9	EU
26	185.3	178.1	T1G	88	587.4	564.7	T2G	150	1013.8	974.6	A1G	212	1597.6	1535.8	T1U
27	185.3	178.1	T1G	89	587.4	564.7	T2G	151	1123.1	1079.7	A2U	213	1597.6	1535.8	T1U
28	193.1	185.7	T1G	90	618.0	594.1	T2U	152	1128.9	1085.2	T2G	214	1597.6	1535.8	T1U</

38	237.0	227.8	T2G	100	705.1	677.8	T1U	162	1138.6	1094.5	T1G	224	3224.7	3099.9	EU
39	238.3	229.1	T1U	101	705.1	677.8	T1U	163	1145.9	1101.6	T2G	225	3225.0	3100.2	T2G
40	238.3	229.1	T1U	102	713.0	685.4	A1G	164	1145.9	1101.6	T2G	226	3225.0	3100.2	T2G
41	238.3	229.1	T1U	103	792.4	761.7	EU	165	1145.9	1101.6	T2G	227	3225.0	3100.2	T2G
42	259.1	249.0	T2U	104	792.4	761.7	EU	166	1146.6	1102.2	T1U	228	3225.8	3101.0	T1G
43	259.1	249.0	T2U	105	793.3	762.6	T1G	167	1146.6	1102.2	T1U	229	3225.8	3101.0	T1G
44	259.1	249.0	T2U	106	793.3	762.6	T1G	168	1146.6	1102.2	T1U	230	3225.8	3101.0	T1G
45	272.7	262.1	EG	107	793.3	762.6	T1G	169	1146.9	1102.5	T2U	231	3226.0	3101.1	A2U
46	272.7	262.1	EG	108	796.1	765.3	T2G	170	1146.9	1102.5	T2U	232	3226.0	3101.2	T2U
47	381.6	366.8	T2G	109	796.1	765.3	T2G	171	1146.9	1102.5	T2U	233	3226.0	3101.2	T2U
48	381.6	366.8	T2G	110	796.1	765.3	T2G	172	1147.8	1103.4	EG	234	3226.0	3101.2	T2U
49	381.6	366.8	T2G	111	796.2	765.4	T1U	173	1147.8	1103.4	EG	235	3226.4	3101.5	T1U
50	386.3	371.3	T1U	112	796.2	765.4	T1U	174	1147.9	1103.4	A1G	236	3226.4	3101.5	T1U
51	386.3	371.3	T1U	113	796.2	765.4	T1U	175	1282.1	1232.5	A1U	237	3226.4	3101.5	T1U
52	386.3	371.3	T1U	114	798.1	767.2	T2U	176	1284.9	1235.2	T1G	238	3226.9	3102.1	T2G
53	398.6	383.2	EG	115	798.1	767.2	T2U	177	1284.9	1235.2	T1G	239	3226.9	3102.1	T2G
54	398.6	383.2	EG	116	798.1	767.2	T2U	178	1284.9	1235.2	T1G	240	3226.9	3102.1	T2G
55	400.4	384.9	T2U	117	799.3	768.4	EG	179	1287.5	1237.7	T2U	241	3227.5	3102.6	EG
56	400.4	384.9	T2U	118	799.3	768.4	EG	180	1287.5	1237.7	T2U	242	3227.5	3102.6	EG
57	400.4	384.9	T2U	119	890.4	856.0	A2U	181	1287.5	1237.7	T2U	243	3228.1	3103.2	T1U
58	406.6	390.8	A2U	120	898.0	863.2	T2G	182	1290.0	1240.1	A2G	244	3228.1	3103.2	T1U
59	406.6	390.9	A1U	121	898.0	863.2	T2G	183	1321.1	1269.9	A1U	245	3228.1	3103.2	T1U
60	408.5	392.7	A1G	122	898.0	863.2	T2G	184	1323.4	1272.2	T1G	246	3228.6	3103.7	A1G
61	417.2	401.1	T1G	123	906.2	871.1	T1U	185	1323.4	1272.2	T1G				
62	417.2	401.1	T1G	124	906.2	871.1	T1U	186	1323.4	1272.2	T1G				