

APPENDIX I

Table A1. Calculated vibrational frequencies (ν , in cm^{-1}) and relative mode Grüneisen parameters (γ_i) of sapphirine-442 ($\text{Mg}_4\text{Al}_8\text{Si}_2\text{O}_{20}$).

N	ν (cm^{-1})	Mode	γ_i	N	ν (cm^{-1})	Mode	γ_i	N	ν (cm^{-1})	Mode	γ_i
1	62.0	Acoustic	1.0	137	358.8	B _g	1.6	273	564.6	B _g	1.0
2	68.9	Acoustic	1.0	138	361.0	B _g	1.2	274	566.2	A _u	0.8
3	111.1	Acoustic	1.0	139	361.5	A _g	1.3	275	568.8	A _g	0.6
4	96.9	A _g	2.2	140	361.7	A _u	1.6	276	572.6	B _u	0.9
5	101.7	A _u	1.3	141	362.8	B _g	1.5	277	574.9	A _u	0.8
6	129.9	A _g	0.7	142	365.2	B _u	1.4	278	576.2	B _g	0.8
7	140.1	A _u	0.4	143	365.3	A _g	1.6	279	577.1	B _g	0.9
8	156.2	B _u	0.5	144	367.4	A _u	1.5	280	577.8	A _u	0.7
9	162.4	A _g	1.3	145	368.2	A _u	1.5	281	580.5	A _u	0.8
10	165.5	B _g	1.2	146	368.7	B _u	1.2	282	585.0	B _u	0.8
11	167.6	B _g	1.0	147	369.4	B _g	1.3	283	585.4	B _g	1.0
12	170.0	A _g	1.0	148	370.2	A _u	1.4	284	586.9	A _g	0.9
13	170.7	A _u	0.5	149	372.9	A _g	1.4	285	591.3	B _g	0.8
14	175.0	B _u	0.7	150	373.0	B _g	1.5	286	592.3	B _u	0.8
15	175.0	B _g	0.8	151	373.1	B _u	1.4	287	592.4	A _u	0.9
16	175.6	A _u	0.8	152	373.3	A _u	1.2	288	595.1	A _g	0.9
17	176.7	A _g	1.2	153	375.7	A _u	1.1	289	595.4	A _u	0.8
18	177.2	B _u	1.8	154	376.0	B _g	1.1	290	596.1	B _u	0.8
19	188.9	B _g	1.1	155	377.7	A _g	0.9	291	597.8	B _g	0.8
20	189.0	A _u	1.2	156	378.8	B _g	1.4	292	601.1	A _g	0.8
21	190.2	B _u	0.8	157	379.1	A _u	1.4	293	604.5	A _g	1.1
22	191.8	B _g	1.5	158	380.7	A _g	1.3	294	604.9	B _u	1.1
23	193.0	A _g	1.0	159	381.2	B _u	1.2	295	606.4	A _u	0.9
24	194.4	B _u	0.5	160	384.2	B _u	1.2	296	610.4	B _g	0.8
25	200.4	B _g	1.0	161	385.2	B _g	1.1	297	610.8	A _u	1.0
26	200.9	A _g	0.9	162	385.7	A _g	1.2	298	615.4	B _u	0.8
27	201.1	B _u	0.7	163	387.2	A _u	1.3	299	617.9	A _g	0.8
28	205.6	A _g	0.7	164	387.5	B _g	1.4	300	624.0	A _g	0.8
29	205.9	B _u	0.9	165	389.3	B _u	1.5	301	625.2	A _u	0.9
30	206.1	B _g	0.7	166	389.9	A _u	1.3	302	627.5	B _u	0.8
31	207.1	A _u	0.7	167	390.1	A _g	1.4	303	629.2	B _g	0.9
32	207.8	A _u	0.9	168	391.5	B _g	1.7	304	629.9	B _g	0.9
33	210.2	B _g	0.7	169	394.2	B _u	1.4	305	636.2	A _u	0.8
34	211.0	B _u	0.5	170	395.1	A _g	1.4	306	642.9	B _u	0.9
35	213.5	A _g	1.3	171	395.2	A _u	1.2	307	643.6	A _g	1.0
36	217.9	A _u	0.5	172	396.4	B _g	1.0	308	645.5	B _g	0.9
37	219.2	A _g	1.0	173	397.2	B _u	1.1	309	649.6	B _u	0.8
38	221.9	B _u	1.3	174	398.1	A _u	1.2	310	656.0	A _u	1.0
39	225.4	B _g	1.1	175	399.8	B _g	1.2	311	657.7	A _g	0.7
40	230.6	A _u	1.2	176	401.1	A _g	1.3	312	661.7	A _g	0.8
41	230.6	A _g	0.6	177	403.9	B _u	1.6	313	663.2	A _u	0.8
42	231.5	B _g	1.2	178	404.1	A _g	1.5	314	666.4	B _u	0.8
43	233.1	B _u	1.0	179	406.3	B _g	1.2	315	667.1	B _g	0.8
44	235.4	B _u	0.5	180	407.3	A _u	1.2	316	672.2	A _g	0.8
45	237.1	A _g	1.1	181	413.7	A _g	1.4	317	673.8	A _u	0.9
46	239.1	B _g	1.1	182	413.9	B _g	1.1	318	675.7	B _u	0.7
47	240.1	A _u	1.1	183	414.5	A _u	1.0	319	678.2	B _g	1.0

48	241.8	B _g	1.2	184	415.6	A _u	1.2	320	683.7	B _g	0.9
49	242.9	A _u	0.8	185	416.8	B _u	1.1	321	685.6	B _u	0.9
50	244.7	A _u	0.7	186	417.6	B _g	1.0	322	691.0	A _g	0.9
51	246.3	A _g	1.7	187	418.3	B _u	1.4	323	691.3	B _g	0.9
52	246.4	B _u	1.7	188	418.5	A _u	1.1	324	694.9	A _g	0.8
53	249.0	B _g	1.1	189	421.0	B _g	1.2	325	697.3	B _u	1.2
54	249.8	A _g	1.2	190	423.0	A _u	1.0	326	700.1	A _g	1.1
55	250.4	A _u	0.8	191	423.2	B _u	1.1	327	702.7	A _u	0.9
56	252.4	B _u	1.3	192	423.4	A _g	0.8	328	702.7	B _u	0.8
57	253.8	B _g	0.9	193	424.4	A _u	1.1	329	704.5	A _u	0.8
58	257.6	B _g	1.2	194	424.7	B _g	1.0	330	707.5	B _g	0.9
59	258.8	B _u	1.0	195	426.6	A _g	1.0	331	713.2	A _g	0.9
60	259.4	A _u	1.4	196	428.1	A _g	1.5	332	721.8	A _u	1.0
61	260.4	A _g	1.2	197	428.4	B _u	1.5	333	723.1	B _g	1.0
62	260.4	B _g	1.1	198	431.3	B _g	1.1	334	727.3	B _u	1.0
63	262.6	A _g	1.2	199	431.9	A _u	0.9	335	727.9	A _u	1.0
64	263.2	A _u	0.9	200	432.1	A _g	1.5	336	729.9	A _g	1.0
65	263.2	B _g	1.3	201	434.7	A _u	1.0	337	730.8	B _u	1.0
66	264.9	A _u	1.4	202	435.5	B _g	1.4	338	732.6	B _g	1.1
67	266.0	B _u	1.5	203	436.1	B _u	1.3	339	734.9	A _g	1.1
68	266.0	A _g	1.1	204	441.1	B _u	1.1	340	737.2	B _g	1.0
69	267.8	B _g	1.3	205	441.8	A _u	1.1	341	740.3	A _u	1.0
70	268.7	B _u	1.1	206	443.5	A _g	1.2	342	741.2	B _u	1.0
71	269.9	A _u	0.9	207	445.7	B _g	1.2	343	746.8	A _g	1.1
72	272.4	B _g	1.1	208	450.2	B _g	1.3	344	747.0	A _u	1.1
73	274.0	A _g	1.9	209	450.7	B _u	1.3	345	748.4	B _u	0.9
74	274.5	B _g	1.3	210	452.5	B _u	1.2	346	750.8	A _g	0.8
75	275.6	A _u	1.1	211	453.1	B _g	0.9	347	751.6	B _g	0.8
76	275.8	B _u	0.9	212	453.2	A _g	1.1	348	752.3	B _u	1.1
77	277.3	B _g	1.1	213	456.5	A _g	1.2	349	756.2	A _u	1.0
78	278.8	A _g	1.0	214	460.0	A _u	0.9	350	757.2	A _u	1.0
79	281.3	B _u	1.4	215	460.1	B _u	1.1	351	766.4	B _g	0.8
80	282.5	A _u	1.3	216	461.4	A _g	1.3	352	766.8	B _g	1.0
81	286.1	A _g	1.1	217	461.9	A _u	1.1	353	773.3	A _g	1.0
82	287.6	B _g	1.0	218	462.0	B _g	0.9	354	773.3	B _u	1.0
83	287.8	A _g	1.1	219	464.2	A _u	1.2	355	780.2	B _g	0.9
84	288.2	B _u	0.8	220	464.7	A _g	1.1	356	780.9	A _u	0.9
85	288.6	A _u	1.0	221	467.9	B _g	1.0	357	789.2	B _u	0.9
86	289.6	A _g	1.3	222	468.7	A _u	1.1	358	797.4	A _g	0.9
87	289.7	B _u	1.1	223	470.4	A _g	0.9	359	804.0	A _g	1.0
88	291.1	A _u	2.0	224	471.2	A _g	1.1	360	813.8	A _u	0.9
89	295.1	A _u	1.5	225	471.6	A _u	1.3	361	816.2	B _g	0.9
90	295.8	B _u	1.1	226	471.7	B _g	1.1	362	817.9	B _u	0.9
91	297.5	B _u	1.2	227	472.5	B _u	1.1	363	824.3	B _u	0.9
92	299.2	A _g	1.1	228	473.2	B _u	1.1	364	825.1	B _g	0.9
93	299.2	A _u	1.0	229	479.9	B _g	0.9	365	826.1	A _u	0.9
94	299.3	B _g	1.2	230	483.1	A _g	1.2	366	826.5	A _g	0.9
95	301.0	A _g	1.2	231	483.3	B _u	0.9	367	833.0	B _g	0.9
96	303.4	B _g	1.2	232	483.4	A _u	0.8	368	835.0	A _u	0.9
97	303.9	B _u	1.0	233	489.6	B _u	1.1	369	843.2	A _g	0.9
98	304.6	A _u	1.3	234	492.4	A _u	0.7	370	843.5	B _g	0.9
99	307.4	B _u	1.0	235	494.2	B _u	1.2	371	843.9	A _u	0.9
100	309.6	B _g	1.3	236	494.6	A _g	1.0	372	850.3	B _u	0.9
101	310.0	A _u	1.6	237	495.2	B _g	1.2	373	867.1	B _u	0.9
102	311.7	A _g	0.7	238	499.5	A _u	0.8	374	867.8	B _g	0.8
103	314.7	A _g	0.9	239	500.9	A _g	1.0	375	869.5	A _u	0.8
104	316.4	B _u	1.2	240	503.4	B _g	0.8	376	870.5	A _g	0.7

105	318.4	B _g	0.7	241	504.1	B _u	0.9	377	874.7	A _g	0.9
106	318.7	A _u	1.2	242	507.2	A _u	1.1	378	876.8	A _u	0.9
107	319.4	B _g	1.1	243	507.9	B _g	0.9	379	888.5	B _u	0.7
108	319.8	B _u	0.9	244	511.5	B _u	1.0	380	892.9	B _u	0.9
109	322.0	A _g	0.8	245	512.7	A _u	1.0	381	894.4	B _g	0.7
110	323.0	A _g	1.3	246	514.3	A _g	1.2	382	902.7	A _u	0.7
111	323.2	B _g	1.1	247	514.6	B _g	0.9	383	903.2	A _g	0.7
112	324.1	A _u	1.7	248	516.0	B _g	1.0	384	909.3	B _g	0.9
113	324.6	B _u	1.7	249	518.5	A _g	1.1	385	920.5	B _g	0.4
114	326.8	A _g	1.5	250	523.9	A _u	0.9	386	922.9	A _g	0.5
115	327.3	A _u	1.5	251	524.4	B _u	0.9	387	935.4	B _u	0.6
116	329.9	B _u	1.7	252	525.9	B _u	1.1	388	936.0	A _u	0.6
117	329.9	B _g	1.8	253	529.8	A _g	1.1	389	941.4	B _u	0.4
118	332.3	A _g	0.9	254	530.6	B _g	0.7	390	946.2	A _u	0.5
119	333.0	B _u	1.3	255	535.6	B _u	0.8	391	955.7	A _g	0.6
120	333.1	A _u	1.4	256	538.5	A _u	0.8	392	961.1	B _g	0.6
121	333.9	A _g	1.4	257	539.1	A _g	0.7	393	973.8	A _u	0.6
122	334.3	B _g	1.6	258	540.7	B _u	0.8	394	974.4	B _u	0.6
123	335.4	B _u	1.2	259	542.0	A _g	0.9	395	978.5	A _u	0.6
124	335.9	A _u	0.9	260	546.7	B _u	0.8	396	978.9	A _g	0.6
125	337.7	A _u	1.6	261	548.3	B _g	0.8	397	979.6	B _g	0.6
126	338.4	A _g	1.6	262	549.9	A _g	0.8	398	981.8	B _u	0.6
127	339.3	B _u	1.5	263	551.9	B _g	0.8	399	988.3	A _g	0.6
128	341.1	B _g	1.1	264	553.1	B _u	0.7	400	995.0	B _u	0.6
129	343.5	B _u	1.4	265	553.8	A _u	0.9	401	995.4	A _u	0.6
130	344.4	B _g	1.4	266	556.1	A _g	0.6	402	1002.0	B _g	0.6
131	346.0	A _g	1.2	267	557.0	B _g	0.8	403	1006.8	A _g	0.6
132	348.7	A _u	1.3	268	557.4	A _g	0.9	404	1011.8	A _u	0.6
133	350.5	A _g	1.1	269	558.1	B _u	0.8	405	1013.1	B _g	0.6
134	353.8	B _u	0.9	270	559.0	A _u	0.8	406	1023.5	A _g	0.6
135	357.3	A _g	1.2	271	561.6	A _g	0.9	407	1040.9	B _g	0.6
136	357.5	B _u	1.5	272	563.6	B _u	0.9	408	1050.6	B _u	0.6

Table A2. Calculated vibrational frequencies (ν_i in cm^{-1}) and relative mode Grüneisen parameters (γ_i) of sapphirine-351 ($\text{Mg}_3\text{Al}_{10}\text{SiO}_{20}$).

N	$\nu (\text{cm}^{-1})$	Mode	γ_i	N	$\nu (\text{cm}^{-1})$	Mode	γ_i	N	$\nu (\text{cm}^{-1})$	Mode	γ_i
1	63.5	Acoustic	1.0	137	363.9	B _g	1.6	273	577.0	B _g	1.0
2	71.4	Acoustic	1.0	138	366.4	B _g	1.6	274	579.6	A _u	0.8
3	114.9	Acoustic	1.0	139	367.1	B _u	1.1	275	581.8	B _u	1.1
4	103.6	A _g	1.6	140	368.2	A _g	1.2	276	582.8	B _g	0.8
5	108.1	A _u	1.2	141	369.5	A _u	1.2	277	583.4	A _g	0.8
6	136.1	A _g	0.7	142	370.1	B _u	1.6	278	585.8	A _u	1.0
7	142.8	A _u	0.3	143	374.8	A _u	1.5	279	586.4	A _g	0.9
8	153.1	B _u	0.2	144	375.3	A _g	1.0	280	592.7	B _g	1.0
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47	243.4	A _u	0.8	183	420.0	A _u	1.0	319	686.1	A _u	1.1
48	245.7	B _g	1.0	184	420.2	B _g	1.2	320	689.2	B _g	1.0
49	247.7	A _u	0.7	185	423.9	B _u	1.4	321	691.9	A _g	0.9
50	251.2	A _u	0.4	186	425.0	A _u	1.1	322	696.4	B _u	1.1
51	254.3	A _g	0.7	187	427.3	B _g	1.1	323	697.7	A _u	1.1

52	255.2	B _g	1.0	188	430.3	A _u	1.2	324	701.8	B _u	1.2
53	255.7	B _u	1.7	189	430.6	B _g	1.1	325	702.3	A _g	1.2
54	257.1	B _g	0.7	190	432.4	B _u	1.1	326	705.3	A _u	1.1
55	257.9	A _u	0.8	191	432.5	A _g	1.2	327	706.2	B _u	1.0
56	259.9	B _u	0.5	192	436.0	A _u	1.4	328	709.8	B _g	1.1
57	260.2	B _g	0.9	193	436.8	B _g	1.0	329	710.5	A _g	1.1
58	260.6	A _u	0.7	194	436.9	A _g	1.2	330	713.5	B _g	1.1
59	261.8	A _g	1.6	195	438.1	A _u	1.2	331	714.4	A _g	1.1
60	262.7	A _u	0.5	196	438.2	B _u	1.2	332	715.2	A _u	1.1
61	264.8	B _u	1.2	197	440.0	B _g	1.4	333	719.9	B _u	1.1
62	266.3	B _g	1.0	198	443.1	A _u	1.1	334	721.0	A _g	1.1
63	267.0	A _g	1.1	199	445.5	A _g	1.2	335	721.1	A _u	1.0
64	268.5	A _g	1.0	200	446.6	B _u	1.3	336	722.9	B _g	1.1
65	269.2	B _u	0.8	201	446.9	A _u	1.3	337	725.2	B _g	1.1
66	271.8	B _g	1.5	202	448.4	B _g	1.0	338	725.8	A _g	1.0
67	272.4	B _u	1.1	203	451.8	A _g	1.3	339	728.8	B _u	1.1
68	273.7	A _g	1.4	204	453.5	B _u	1.0	340	731.4	A _u	1.2
69	274.4	B _g	1.1	205	453.9	A _u	1.2	341	733.6	B _u	1.1
70	274.5	A _u	1.2	206	454.4	B _g	1.1	342	733.6	B _g	1.0
71	277.1	A _u	1.0	207	456.2	A _u	1.2	343	733.9	A _g	1.1
72	279.4	B _u	0.9	208	458.8	A _g	1.1	344	738.0	B _u	1.2
73	279.6	A _g	0.7	209	459.5	B _g	1.3	345	741.0	B _g	1.1
74	281.2	B _g	1.2	210	461.1	A _g	1.1	346	745.5	A _u	1.0
75	281.3	A _u	0.7	211	463.4	B _u	1.2	347	746.0	A _g	1.1
76	282.7	A _g	1.2	212	464.9	A _u	1.1	348	747.1	B _g	1.2
77	282.9	B _g	1.0	213	465.4	A _g	1.0	349	748.5	B _u	1.1
78	285.1	A _u	1.6	214	465.9	B _g	1.3	350	749.7	A _u	1.0
79	285.2	B _u	1.0	215	466.6	B _u	1.3	351	752.8	B _g	1.0
80	290.3	A _g	1.4	216	467.5	A _u	1.2	352	754.7	A _g	1.1
81	292.2	B _g	1.1	217	470.6	B _g	1.1	353	757.6	B _u	1.0
82	293.3	B _u	1.3	218	471.3	A _g	0.9	354	760.7	A _u	1.0
83	293.4	A _g	1.3	219	476.0	A _g	1.4	355	766.0	A _g	1.1
84	294.5	B _g	1.3	220	477.0	B _g	1.2	356	774.9	B _g	1.0
85	297.5	A _g	1.3	221	478.7	B _u	1.2	357	780.0	A _u	1.0
86	297.9	A _u	1.3	222	480.1	A _u	1.2	358	780.6	B _u	1.0
87	298.4	B _u	0.9	223	480.2	B _u	1.6	359	780.6	A _u	1.2
88	301.5	A _g	1.4	224	481.2	A _g	1.5	360	781.4	B _g	1.0
89	301.6	B _u	0.8	225	481.7	B _g	1.1	361	782.4	A _g	1.1
90	303.7	A _u	1.1	226	485.8	A _u	0.8	362	794.7	B _u	1.1
91	305.0	A _u	1.5	227	488.3	B _u	1.2	363	798.1	A _u	1.0
92	306.9	B _g	0.7	228	491.3	A _g	1.1	364	802.8	A _g	1.0
93	307.0	B _u	1.1	229	492.9	B _g	1.0	365	804.5	B _u	1.1
94	307.4	A _g	1.0	230	494.8	B _u	1.0	366	806.9	B _g	1.0
95	308.4	B _g	1.1	231	495.8	A _u	1.1	367	809.8	A _u	1.0
96	309.4	B _u	1.0	232	497.7	A _u	0.9	368	812.2	B _u	1.0
97	310.7	A _g	1.0	233	500.2	A _g	1.2	369	821.8	B _g	0.9
98	311.1	A _u	1.5	234	500.7	B _u	1.3	370	825.6	A _g	1.0
99	313.4	A _u	1.3	235	504.7	B _g	1.0	371	829.3	A _u	1.0
100	314.7	B _u	0.7	236	505.5	B _g	1.3	372	833.0	B _u	0.9
101	319.2	B _g	1.0	237	506.2	A _g	1.3	373	833.1	B _g	0.9
102	319.4	A _g	1.1	238	508.2	A _u	1.0	374	835.2	B _g	0.9
103	320.7	A _u	1.2	239	510.3	A _g	1.2	375	839.0	A _u	1.0
104	321.5	B _u	1.5	240	511.6	B _u	1.0	376	840.3	A _g	0.9
105	322.3	B _g	1.1	241	515.1	B _u	1.2	377	846.6	B _g	0.9
106	323.4	B _u	1.2	242	515.2	B _g	1.0	378	847.2	B _u	0.9
107	325.2	B _g	1.1	243	516.9	A _u	1.2	379	848.7	A _u	0.9
108	325.6	A _g	0.9	244	519.4	A _g	1.0	380	852.3	B _u	0.9

109	328.1	A _g	0.9	245	520.3	A _u	1.1	381	855.3	A _g	0.9
110	328.2	A _u	0.9	246	520.7	B _g	1.1	382	857.5	A _u	0.9
111	330.9	A _g	1.4	247	521.4	B _u	1.0	383	860.3	A _g	0.7
112	331.1	A _u	1.8	248	523.9	B _g	0.8	384	866.9	A _g	0.9
113	334.6	B _u	1.3	249	526.2	B _u	1.0	385	871.6	A _u	0.8
114	334.7	A _u	1.1	250	527.6	A _g	1.5	386	876.4	B _u	0.8
115	334.8	B _g	1.0	251	531.8	B _u	1.3	387	877.4	B _g	0.8
116	336.1	B _u	1.5	252	533.8	A _g	1.0	388	878.6	B _g	0.8
117	336.6	A _u	1.4	253	536.0	A _u	1.0	389	884.3	A _g	0.8
118	337.6	A _g	1.1	254	536.2	A _g	1.0	390	889.0	A _u	0.8
119	338.5	B _u	1.6	255	538.4	B _u	1.1	391	896.3	B _u	0.7
120	339.1	B _g	1.8	256	538.6	A _u	1.0	392	908.2	A _u	0.7
121	340.8	A _u	1.5	257	542.2	A _g	0.9	393	911.0	B _g	0.7
122	341.1	B _u	2.0	258	545.6	B _u	0.9	394	913.1	B _u	0.7
123	341.9	A _g	1.1	259	546.9	A _g	1.0	395	916.3	A _g	0.6
124	344.5	B _g	1.3	260	546.9	B _g	1.0	396	923.5	B _g	0.7
125	345.8	B _u	1.4	261	550.1	B _u	0.8	397	932.3	B _u	0.6
126	346.3	B _g	1.5	262	550.3	B _g	0.8	398	937.0	A _u	0.6
127	346.7	A _u	1.3	263	555.6	B _u	0.8	399	968.8	A _g	0.6
128	348.9	A _u	1.7	264	557.7	B _g	0.9	400	970.7	A _g	0.6
129	349.4	A _g	1.5	265	561.7	A _u	1.0	401	974.1	B _g	0.6
130	352.0	A _g	1.6	266	563.1	B _u	0.7	402	977.2	A _u	0.6
131	357.0	B _u	1.2	267	564.3	A _u	0.9	403	980.0	B _u	0.6
132	357.1	B _g	1.1	268	564.3	A _g	0.8	404	985.4	B _g	0.7
133	360.1	A _g	1.2	269	567.8	A _g	0.8	405	990.1	A _u	0.6
134	360.1	B _g	1.2	270	570.2	B _g	1.0	406	992.7	A _g	0.6
135	361.4	A _u	1.4	271	573.8	B _u	1.0	407	1000.4	B _g	0.6
136	363.2	B _u	1.0	272	574.4	A _u	1.0	408	1019.0	B _u	0.6