APPENDIX 1

Representative EMP composition of boracite and temperatures of phase transition

Crystal B1										
Analysis #	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**
MgO	29.90	30.20	30.06	30.44	30.95	30.36	29.73	30.10	30.63	30.30
FeO	1.31	0.02	0.00	0.38	0.01	0.07	1.90	0.09	0.12	0.88
MnO	0.19	0.00	0.00	0.02	0.02	0.00	0.08	0.00	0.00	0.16
Cl	9.00	8.94	9.03	9.06	9.31	9.19	9.12	9.28	9.10	9.12
B_2O_3	61.97	60.85	60.52	61.78	62.31	61.18	62.14	60.62	61.82	62.23
$O = Cl_2$	–2.03	–2.02	–2.04	–2.04	–2.10	–2.07	–2.06	–2.09	–2.05	–2.06
Total	100.34	97.99	97.58	99.64	100.49	98.73	100.92	97.99	99.61	100.63
Number of ions on the basis of 3 Me^{2+} and 14 (O.Cl) pfu										
Mg	2.92	3.00	3.00	2.98	3.00	3.00	2.89	3.00	2.99	2.94
Fe	0.07	0.00	0.00	0.02	0.00	0.00	0.10	0.00	0.01	0.05
Mn	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
B	7.00	7.00	6.99	7.00	6.99	6.99	7.00	6.98	7.00	7.00
Cl	1.00	1.01	1.02	1.01	1.03	1.03	1.01	1.02	1.01	1.01
Temperatures of transition ($Pca2_1$)→(F43c)	**269.4°C**	**268.2°C**	**264°C**	**255°C**	**240°C**	**269.4°C**	**271°C**	**269°C**	**264°C**	**269.8°C**
Crystal B2										
Analysis #	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
MgO	30.11	29.02	30.46	28.97	25.46	29.74	30.82	30.46	30.65	30.13
FeO	0.51	2.05	0.01	2.42	7.42	1.53	0.07	0.12	0.11	0.02
MnO	0.02	0.11	0.02	0.20	0.25	0.06	0.00	0.00	0.05	0.02
Cl	9.07	8.97	8.99	8.94	8.72	9.00	9.16	9.12	9.12	8.89
B_2O_3	61.23	60.89	61.41	61.01	60.00	61.72	62.14	61.47	61.91	60.74
$O = Cl_2$	–2.05	–2.02	–2.03	–2.00	–1.97	–2.03	–2.07	–2.06	–2.06	–2.01
Total	98.90	99.01	98.86	100.00	99.89	100.02	100.12	99.11	99.78	97.79
Number of ions on the basis of 3 Me^{2+} and 14 (O.Cl) pfu										
Mg	2.97	2.88	3.00	2.86	2.57	2.91	3.00	2.99	2.99	3.00
Fe	0.03	0.11	0.00	0.13	0.42	0.08	0.00	0.01	0.01	0.00
Mn	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00
B	6.99	7.00	7.00	7.00	7.00	7.00	7.00	6.99	7.00	7.00
Cl	1.02	1.01	1.01	1.00	1.00	1.00	1.01	1.02	1.01	1.01
Temperatures of transition ($Pca2_1$)→(F43c)	**269°C**	**270°C**	**269°C**	**270.5°C**	**271°C**	**272°C**	**262°C**	**263°C**	**269°C**	**265°C**
Crystal B3										
Analysis #	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
MgO	30.67	30.46	30.75	29.67	29.51	30.95	30.96	29.84	30.79	30.25
FeO	0.07	0.12	0.05	1.22	1.77	0.11	0.11	1.45	0.12	0.04
MnO	0.02	0.02	0.01	0.06	0.02	0.01	0.04	0.12	0.02	0.00
Cl	9.16	9.07	8.92	9.15	8.98	9.00	9.12	8.97	8.97	9.00
B_2O_3	61.86	61.51	62.09	61.17	61.49	62.54	62.56	61.93	62.24	60.97
$O = Cl_2$	–2.07	–2.05	–2.01	–2.06	–2.03	–2.03	–2.06	–2.02	–2.02	–2.03
Total	99.72	99.13	99.81	99.20	99.75	100.57	100.73	100.28	100.11	98.23
Number of ions on the basis of 3 Me^{2+} and 14 (O.Cl) pfu										
Mg	3.00	2.99	3.00	2.93	2.90	2.99	2.99	2.91	2.99	3.00
Fe	0.00	0.01	0.00	0.07	0.10	0.01	0.01	0.08	0.01	0.00
Mn	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
B	6.99	7.00	7.00	6.99	7.00	7.00	7.00	7.00	7.00	7.00
Cl	1.02	1.01	0.99	1.03	1.00	0.99	1.00	1.00	0.99	1.01
Temperatures of transition ($Pca2_1$)→(F43c)	**266°C**	**268.6°C**	**210°C**	**269°C**	**269.8°C**	**269°C**	**230°C**	**269°C**	**268.8°C**	**264°C**