Supplemental Tables

TABLE OM1. Complete calculated X-ray powder diffraction data (Cu$K\alpha$) for alumino-oxy-rossmanite.

h	k	l	$d_{calc.}$	$I_{calc.}$
1	1	0	7.9015	2
1	**0**	**1**	**6.2938**	**28**
0	2	1	4.9229	23
0	3	0	4.5620	17
2	**1**	**1**	**4.1783**	**61**
2	**2**	**0**	**3.9508**	**85**
0	**1**	**2**	**3.4307**	**55**
1	3	1	3.3461	15
4	0	1	3.0812	4
1	4	0	2.9865	17
1	**2**	**2**	**2.9236**	**78**
3	2	1	2.8707	8
3	3	0	2.6338	2
3	1	2	2.5904	7
0	**5**	**1**	**2.5534**	**100**
2	4	1	2.4297	4
0	0	3	2.3626	10
2	3	2	2.3501	13
5	1	1	2.3224	22
0	6	0	2.2810	2
5	0	2	2.1663	9
4	3	1	2.1445	13
0	3	3	2.0979	6
3	0	3	2.0979	5
4	2	2	2.0892	7
2	2	3	2.0277	12
1	**5**	**2**	**2.0198**	**39**
1	6	1	2.0021	8
4	4	0	1.9754	2
3	**4**	**2**	**1.8995**	**30**
3	5	1	1.8847	2
1	4	3	1.8529	5
6	2	1	1.8333	8
3	3	3	1.7587	6
1	0	4	1.7573	3
0	2	4	1.7154	2
2	6	2	1.6731	4
0	6	3	1.6410	16

6	0	3	1.6410	3
2	7	1	1.6273	12
5	5	0	1.5803	14
4	0	4	1.5734	3
4	5	2	1.5708	4
8	1	1	1.5624	3
3	2	4	1.5431	2

Notes: Calculated using single-crystal structural data of sample PINK1. Only reflections with $I_{calc} > 1$ are listed. The eight strongest reflections are in bold.

TABLE OM2. Theoretical compositions of known and potential Al-rich and Li-bearing tourmalines.

	1	2	3	4	5	6	7	8
SiO_2	31.90	38.65	39.03	38.49	38.40	38.12	37.41	38.12
Al_2O_3	54.14	46.45	44.15	40.82	40.73	43.12	47.61	37.73
B_2O_3	11.09	11.20	11.30	11.15	11.12	11.04	10.84	11.04
Li_2O	-	0.80	1.62	2.39	2.39	1.58	-	3.16
Na_2O	-	-	-	3.31	3.30	3.28	3.22	-
CaO	-	-	-	-	-	-	-	5.93
H_2O	2.87	2.90	3.90	3.85	2.88	2.86	0.93	2.86
F	-	-	-	-	2.02	-	-	2.01
X site	□	□	□	Na	Na	Na	Na	Ca
Y site	Al_3	$Al_{2.5}Li_{0.5}$	Al_2Li	$Li_{1.5}Al_{1.5}$	$Li_{1.5}Al_{1.5}$	Al_2Li	Al_3	Li_2Al
Z site	Al_6	Al_6	Al_6	Al_6	Al_6	Al_6	Al_6	Al_6
B site	B_3	B_3	B_3	B_3	B_3	B_3	B_3	B_3
T site	Si_5Al	Si_6	Si_6	Si_6	Si_6	Si_6	Si_6	Si_6
V site	$(OH)_3$	$(OH)_3$	$(OH)_3$	$(OH)_3$	$(OH)_3$	$(OH)_3$	$O_2(OH)^*$	$(OH)_3$
W site	O	O	OH	OH	F	O	O^*	F

Notes: 1: Alumino-oxy-rossmanite, $□Al_3Al_6(Si_5AlO_{18})(BO_3)_3(OH)_3O$; 2 "oxy-rossmanite", $□(Li_{0.5}Al_{2.5})Al_6Si_6O_{18}(BO_3)_3(OH)_3O$; 3: Rossmanite, $□(LiAl_2)Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$; 4: Elbaite, $Na(Li_{1.5}Al_{1.5})Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$; 5: Fluor-elbaite, $Na(Li_{1.5}Al_{1.5})Al_6Si_6O_{18}(BO_3)_3(OH)_3F$; 6: Darrellhenryite, $Na(LiAl_2)Al_6Si_6O_{18}(BO_3)_3(OH)_3O$; 7: Olenite $NaAl_3Al_6Si_6O_{18}(BO_3)_3(O)_3OH$; 8: Fluor-liddicoatite, $Ca(Li_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3F$;

*To produce an ordered end-member formula of olenite, the (OH) group can be assigned to the V site although it occupies the W site.