

Table S1. *Luinaite-(OH)*: sites, fractional atomic coordinates, isotropic (*) or equivalent-isotropic displacement parameters (in Å²), site occupancies (s.o.) for schorl-1A from Cleveland tin mine, Australia (Sample LUI-AUS), and for oxy-dravite-1A from Blue Mountain Saddle, USA (Sample LUI-USA).

Site	Sample LUI-AUS				S.O.
	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>U</i> _{eq/iso}	
X	-0.0008(2)	0.0001(2)	0.2497(4)	0.0241(10)	Na _{0.711(10)}
Ya	0.60395(5)	0.39544(6)	-0.01761(11)	0.0102(2)	Al _{0.475(7)} Fe _{0.525(7)}
Yb	0.79092(6)	0.39574(7)	-0.01598(12)	0.0101(3)	Al _{0.592(7)} Fe _{0.408(7)}
Yc	0.60348(6)	0.20819(7)	-0.01537(12)	0.0097(3)	Al _{0.637(7)} Fe _{0.363(7)}
Za	0.63075(8)	0.70298(9)	0.29721(16)	0.0067(3)	Al _{0.983(6)} Fe _{0.017(6)}
Zb	0.96283(8)	0.70185(9)	0.63019(15)	0.0073(3)	Al _{0.925(6)} Fe _{0.075(6)}
Zc	1.07138(8)	0.70347(9)	0.29740(16)	0.0062(3)	Al _{0.988(6)} Fe _{0.012(6)}
Zd	0.73777(7)	0.70158(8)	0.63009(14)	0.0070(3)	Al _{0.876(6)} Fe _{0.124(6)}
Ze	0.96247(8)	0.26143(9)	0.63078(15)	0.0068(3)	Al _{0.956(6)} Fe _{0.044(6)}
Zf	0.96465(7)	0.59496(8)	-0.03643(14)	0.0067(3)	Al _{0.883(6)} Fe _{0.117(6)}
Ta	0.85779(7)	0.52351(8)	0.35300(15)	0.0070(2)	Si _{1.00}
Tb	0.66397(7)	0.52328(8)	0.35205(15)	0.0069(2)	Si _{1.00}
Tc	0.47666(7)	0.33581(8)	0.35240(15)	0.0069(2)	Si _{1.00}
Td	0.85724(7)	0.33594(8)	0.35409(15)	0.0070(2)	Si _{1.00}
Te	0.66378(7)	0.14232(8)	0.35447(15)	0.0067(2)	Si _{1.00}
Tf	0.47612(7)	0.14201(8)	0.35397(15)	0.0068(2)	Si _{1.00}
B1	0.7800(3)	0.8898(4)	0.4753(6)	0.0093(8)	B _{1.00}
B2	0.7761(3)	0.5528(4)	-0.1925(6)	0.0095(8)	B _{1.00}
B3	0.1092(3)	0.8899(3)	0.4769(6)	0.0087(7)	B _{1.00}
O1A	0.6668(3)	0.3312(3)	0.1290(5)	0.0270(8)	O _{1.00}
O2A	0.5431(2)	0.2697(3)	-0.1559(4)	0.0148(7)	O _{1.00}
O2B	0.7273(2)	0.2714(3)	-0.1527(4)	0.0149(6)	O _{1.00}
O2C	0.7287(2)	0.4553(2)	-0.1572(4)	0.0162(7)	O _{1.00}
O3A	0.5329(2)	0.4659(2)	-0.1365(4)	0.0158(7)	O _{1.00}
H3A	0.543(4)	0.459(5)	-0.265(4)	0.019	H _{1.00}
O3B	0.8696(3)	0.7388(3)	0.5288(4)	0.0190(7)	O _{1.00}
H3B	0.881(4)	0.761(5)	0.403(5)	0.023	H _{1.00}
O3C	0.9282(3)	0.4628(3)	-0.1378(4)	0.0182(7)	O _{1.00}
H3C	0.925(4)	0.465(5)	-0.268(4)	0.022	H _{1.00}
O4A	0.7598(2)	0.5213(2)	0.4223(4)	0.0130(6)	O _{1.00}
O4B	0.4799(2)	0.2408(2)	0.4228(4)	0.0142(6)	O _{1.00}
O4C	0.7578(2)	0.2420(2)	0.4223(4)	0.0128(6)	O _{1.00}
O5A	0.5735(2)	0.4266(2)	0.4436(4)	0.0121(6)	O _{1.00}
O5B	0.5719(2)	0.1462(2)	0.4467(4)	0.0116(6)	O _{1.00}
O5C	0.8529(2)	0.4276(2)	0.4456(4)	0.0125(6)	O _{1.00}
O6A	0.8609(2)	0.5178(2)	0.1302(4)	0.0124(6)	O _{1.00}
O6B	0.6555(2)	0.5195(2)	0.1293(4)	0.0117(6)	O _{1.00}
O6C	0.6551(2)	0.1379(2)	0.1315(4)	0.0111(6)	O _{1.00}
O6D	0.8624(2)	0.3444(2)	0.1308(4)	0.0100(5)	O _{1.00}
O6E	0.4802(2)	0.3442(2)	0.1292(4)	0.0112(6)	O _{1.00}
O6F	0.4812(2)	0.1385(2)	0.1307(4)	0.0121(6)	O _{1.00}
O7A	0.6649(2)	0.6180(2)	0.4285(4)	0.0115(6)	O _{1.00}
O7B	0.9515(2)	0.6197(2)	0.4285(4)	0.0104(6)	O _{1.00}
O7C	0.6682(2)	0.0505(2)	0.4335(4)	0.0117(6)	O _{1.00}
O7D	0.38004(19)	0.0491(2)	0.4309(4)	0.0106(6)	O _{1.00}
O7E	0.3817(2)	0.3342(2)	0.4299(4)	0.0121(6)	O _{1.00}
O7F	0.9491(2)	0.3322(2)	0.4330(4)	0.0119(6)	O _{1.00}
O8A	0.8750(2)	0.6029(2)	-0.2102(5)	0.0137(6)	O _{1.00}
O8B	1.0607(2)	0.7908(2)	0.4587(4)	0.0132(6)	O _{1.00}
O8C	1.2089(2)	0.9394(2)	0.4616(4)	0.0121(6)	O _{1.00}
O8D	0.7286(2)	0.7910(2)	0.4551(5)	0.0133(6)	O _{1.00}
O8E	1.0646(2)	0.6074(2)	0.1296(4)	0.0132(6)	O _{1.00}
O8F	0.0587(2)	0.2686(2)	0.4614(5)	0.0137(6)	O _{1.00}

Sample LUI-USA					
<i>Site</i>	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>U_{eq/iso}</i>	<i>s.o.</i>
X	-0.00038(13)	0.00022(14)	0.2503(2)	0.0243(5)	Na _{0.889(6)}
Ya	0.60436(5)	0.39476(5)	-0.01194(10)	0.0095(2)	Al _{0.751(4)} Fe _{0.249(4)}
Yb	0.78915(5)	0.39479(5)	-0.01212(9)	0.00932(19)	Al _{0.721(4)} Fe _{0.279(4)}
Yc	0.60405(5)	0.20934(6)	-0.01034(10)	0.0089(2)	Al _{0.832(4)} Fe _{0.168(4)}
Za	0.63035(6)	0.70283(6)	0.29618(11)	0.0060(2)	Al _{0.984(4)} Fe _{0.016(4)}
Zb	0.96291(6)	0.70214(6)	0.62925(11)	0.0071(2)	Al _{0.942(4)} Fe _{0.058(4)}
Zc	1.07121(6)	0.70288(6)	0.29591(11)	0.0061(2)	Al _{0.978(4)} Fe _{0.022(4)}
Zd	0.73790(6)	0.70223(6)	0.62895(11)	0.0068(2)	Al _{0.954(4)} Fe _{0.046(4)}
Ze	0.96274(6)	0.26138(6)	0.62907(11)	0.0064(2)	Al _{0.958(4)} Fe _{0.042(4)}
Zf	0.96399(6)	0.59475(6)	-0.03778(11)	0.0066(2)	Al _{0.958(4)} Fe _{0.042(4)}
Ta	0.85775(5)	0.52348(6)	0.35171(10)	0.00635(14)	Si _{1.00}
Tb	0.66422(5)	0.52328(6)	0.35142(10)	0.00675(14)	Si _{1.00}
Tc	0.47711(5)	0.33578(6)	0.35258(10)	0.00693(14)	Si _{1.00}
Td	0.85727(5)	0.33575(6)	0.35300(10)	0.00633(14)	Si _{1.00}
Te	0.66422(5)	0.14240(6)	0.35406(10)	0.00596(14)	Si _{1.00}
Tf	0.47671(5)	0.14236(6)	0.35411(10)	0.00610(14)	Si _{1.00}
B1	0.7795(2)	0.8896(2)	0.4731(5)	0.0095(5)	B _{1.00}
B2	0.7752(2)	0.5518(2)	-0.1942(4)	0.0091(5)	B _{1.00}
B3	0.1088(2)	0.8897(2)	0.4736(4)	0.0085(5)	B _{1.00}
O1A	0.66472(18)	0.33179(19)	0.1225(3)	0.0161(4)	O _{1.00}
O2A	0.54422(15)	0.27123(17)	-0.1545(3)	0.0128(4)	O _{1.00}
O2B	0.72534(16)	0.27064(17)	-0.1543(3)	0.0129(4)	O _{1.00}
O2C	0.72590(17)	0.45408(17)	-0.1576(3)	0.0142(4)	O _{1.00}
O3A	0.53517(16)	0.46166(18)	-0.1361(3)	0.0160(5)	O _{1.00}
H3A	0.538(3)	0.460(3)	-0.267(3)	0.019	H _{1.00}
O3B	0.87167(17)	0.74410(19)	0.5289(3)	0.0173(5)	O _{1.00}
H3B	0.873(3)	0.751(3)	0.402(3)	0.021	H _{1.00}
O3C	0.92600(19)	0.46172(18)	-0.1367(3)	0.0171(5)	O _{1.00}
H3C	0.921(3)	0.459(3)	-0.263(3)	0.02	H _{1.00}
O4A	0.76036(15)	0.52217(17)	0.4240(3)	0.0132(4)	O _{1.00}
O4B	0.48136(17)	0.24129(16)	0.4247(3)	0.0138(4)	O _{1.00}
O4C	0.75847(15)	0.24137(16)	0.4242(3)	0.0129(4)	O _{1.00}
O5A	0.57432(15)	0.42622(16)	0.4445(3)	0.0119(4)	O _{1.00}
O5B	0.57278(14)	0.14724(17)	0.4479(3)	0.0114(4)	O _{1.00}
O5C	0.85062(16)	0.42639(16)	0.4455(3)	0.0117(4)	O _{1.00}
O6A	0.85963(15)	0.51687(17)	0.1294(3)	0.0115(4)	O _{1.00}
O6B	0.65548(15)	0.51660(16)	0.1290(3)	0.0113(4)	O _{1.00}
O6C	0.65564(15)	0.14031(16)	0.1314(3)	0.0102(4)	O _{1.00}
O6D	0.86132(15)	0.34389(16)	0.1302(3)	0.0092(4)	O _{1.00}
O6E	0.48191(15)	0.34421(16)	0.1300(3)	0.0095(4)	O _{1.00}
O6F	0.48337(15)	0.14075(17)	0.1320(3)	0.0107(4)	O _{1.00}
O7A	0.66444(15)	0.61809(15)	0.4259(3)	0.0105(4)	O _{1.00}
O7B	0.95222(14)	0.61841(15)	0.4263(3)	0.0100(4)	O _{1.00}
O7C	0.66808(14)	0.05019(15)	0.4304(3)	0.0101(4)	O _{1.00}
O7D	0.38063(14)	0.04971(16)	0.4300(3)	0.0100(4)	O _{1.00}
O7E	0.38230(14)	0.33404(16)	0.4297(3)	0.0120(4)	O _{1.00}
O7F	0.94974(15)	0.33335(16)	0.4310(3)	0.0123(4)	O _{1.00}
O8A	0.87456(15)	0.60185(17)	-0.2095(3)	0.0132(4)	O _{1.00}
O8B	1.06112(15)	0.79122(16)	0.4552(3)	0.0121(4)	O _{1.00}
O8C	1.20840(14)	0.93999(16)	0.4614(3)	0.0111(4)	O _{1.00}
O8D	0.72902(15)	0.79123(16)	0.4538(3)	0.0123(4)	O _{1.00}
O8E	1.06377(15)	0.60702(16)	0.1282(3)	0.0115(4)	O _{1.00}
O8F	0.05931(15)	0.26889(16)	0.4583(3)	0.0129(4)	O _{1.00}