ATOMIC COORDINATES, DISPLACEMENT PARAMETERS (Å^2), AND OCCUPANCIES FOR THE FAMILY STRUCTURE OF BOULANGERITE.

Site	Atom	s.o.f.	x/a	y/b	z/c	Uiso	U11	U22	U33	U23	U13	U12
A1	Pb	1	0.11732(5)	0.49894(4)	0.25	0.0285(4)	0.0451(5)	0.0213(4)	0.0191(4)	0.000	0.000	-0.0028(4)
A2	Pb	1	0.30675(4)	0.15995(3)	0.25	0.0193(3)	0.0200(3)	0.0232(3)	0.0148(3)	0.000	0.000	-0.0019(3)
A3	Pb	1	0.20628(4)	0.32299(4)	0.25	0.0222(4)	0.0205(3)	0.0286(4)	0.0176(4)	0.000	0.000	0.0005(3)
A4	Pb	0.4853(8)	0.45726(7)	0.43223(6)	0.75	0.0391(7)	0.0526(8)	0.0286(6)	0.0362(7)	0.000	0.000	0.0144(6)
	Sb	0.5147(8)	0.45726(7)	0.43223(6)	0.75	0.0391(7)	0.0526(8)	0.0286(6)	0.0362(7)	0.000	0.000	0.0144(6)
A5	Pb	0.5353(8)	0.13135(5)	0.09796(5)	0.75	0.0280(5)	0.0246(5)	0.0346(6)	0.0249(5)	0.000	0.000	-0.0056(4)
	Sb	0.4648(8)	0.13135(5)	0.09796(5)	0.75	0.0280(5)	0.0246(5)	0.0346(6)	0.0249(5)	0.000	0.000	-0.0056(4)
A6	Sb	0.5	0.37113(13)	0.30838(12)	0.75	0.0164(10)	0.0143(10)	0.0185(11)	0.0163(8)	0.000	0.000	-0.0015(7)
	Sb	0.5	0.38766(13)	0.28409(12)	0.75	0.0164(10)	0.0143(10)	0.0185(11)	0.0163(8)	0.000	0.000	-0.0015(7)
A7	Pb	0.5134(8)	0.04622(9)	0.23259(5)	0.25	0.0425(9)	0.0845(11)	0.0194(5)	0.0237(6)	0.000	0.000	-0.0082(6)
	Sb	0.4866(8)	0.04622(9)	0.23259(5)	0.25	0.0425(9)	0.0845(11)	0.0194(5)	0.0237(6)	0.000	0.000	-0.0082(6)
A8	Pb	0.4821(8)	0.48657(5)	0.12965(5)	0.75	0.0265(5)	0.0203(5)	0.0420(6)	0.0172(5)	0.000	0.000	0.0015(4)
	Sb	0.5180(8)	0.48657(5)	0.12965(5)	0.75	0.0265(5)	0.0203(5)	0.0420(6)	0.0172(5)	0.000	0.000	0.0015(4)
A9	Sb	1	0.28796(7)	0.46188(7)	0.75	0.0271(7)	0.0245(7)	0.0347(8)	0.0220(7)	0.000	0.000	-0.0105(6)
S1	S	1	0.0689(2)	0.0160(2)	0.25	0.0193(2)	0.017(2)	0.022(2)	0.019(2)	0.000	0.000	0.0026(18)
S2	S	1	0.1867(2)	0.4144(2)	0.75	0.0148(2)	0.0135(19)	0.019(2)	0.0117(19)	0.000	0.000	-0.0012(16)
S3	S	1	0.2463(3)	0.0284(2)	0.25	0.0237(2)	0.018(2)	0.023(2)	0.030(3)	0.000	0.000	0.0004(19)
S4	S	1	0.0959(3)	0.2939(3)	0.75	0.0368(3)	0.017(2)	0.022(3)	0.071(5)	0.000	0.000	-0.007(2)
S5	S	1	0.1557(2)	0.1738(2)	0.25	0.0223(2)	0.013(2)	0.020(2)	0.034(3)	0.000	0.000	- 0.0001(17)
S6	S	1	0.3313(3)	0.3742(2)	0.25	0.0301(3)	0.020(2)	0.018(2)	0.052(4)	0.000	0.000	-0.0010(19)
S7	S	1	0.4191(2)	0.2207(2)	0.25	0.0234(2)	0.017(2)	0.021(2)	0.032(3)	0.000	0.000	-0.0016(18)
S8	S	1	0.0136(3)	0.4417(2)	0.75	0.0296(3)	0.015(2)	0.022(2)	0.052(4)	0.000	0.000	0.0006(19)
S9	S	1	0.3714(3)	0.0886(2)	0.75	0.0224(2)	0.028(3)	0.024(2)	0.015(2)	0.000	0.000	0.005(2)
S10	S	1	0.2771(2)	0.2505(2)	0.75	0.0162(2)	0.019(2)	0.018(2)	0.012(2)	0.000	0.000	0.0013(17)
S11	S	1	0.0143(2)	0.1362(2)	0.75	0.0202(2)	0.016(2)	0.020(2)	0.025(3)	0.000	0.000	0.0035(18)

SELECTED BOND DISTANCES (Å) FOR THE FAMILY STRUCTURE OF THE BOULANGERITE.

A1	-S3	2.969(5)	A2 -S7	2.774(5)	A3 -S6	2.907(6)
	-S9	2.925(4)x2	-S	2.958(4)x2	-S2	2.974(4)x2
	-S8	3.102(6)	-S10	2.996(4)x2	-S10	3.036(4)x2
	-S2	3.188(4)x2	-S5	3.213(5)	-S4	3.161(4)x2
	-S8	3.271(4)x2	-S3	3.342(6)		
A4	-S1	2.657(5)	A5 -S11	2.635(5)	A6a –S10	2.410(6)
	-S11	2.849(4)x2	-S5	2.739(4)x2	-S6	2.677(6)x2
	-S1	2.871(4)x2	-S1	3.086(4)x2	-S7	3.056(5)x2
	-S6	3.611(5)x2	-S3	3.557(5)	-S11	3.842(5)x2
A6b	-S10	2.470(6)	A7 -S4	2.693(4)x2	A8 -S7	3.268(4)x2
	-S7	2.594(4)x2	-S5	2.699(5)	-S9	2.622(6)
	-S6	3.157(5)x2	-S11	3.105(4)x2	-S8	2.683(4)x2
	-S11	3.867(5)	-S7	3.537(4)x2	-S4	3.557(5)
A9	-S2	2.416(5)				
	-S3	2.653(4)x2				
	-S6	3.025(4)x2				
	-S1	3.856(4)				