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Supporting Information

Manipulation of Birefringence via Substitution of Sr^{2+} by Pb^{2+} Based on the Structure Model of $LiSr_{1-x}Pb_xBO_3$ ($0 \leq x \leq 0.5$)

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Table S1 Selected bond lengths (Å) for $LiSr_{1-x}Pb_xBO_3$ (x=0.138, 0.285, 0.320, 0.379, 0.417, 0.5)

Bond	Bond Lengths	Bond	bond lengths
	$LiSr_{0.862}Pb_{0.138}BO_3$		
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.471(7)	Li(1)-O(2)$^{\#5}$	1.941(13)
Sr(1)/Pb(1)-O(2)	2.523(7)	Li(1)-O(3)	1.965(13)
Sr(1)/Pb(1)-O(2)$^{\#2}$	2.531(7)	Li(1)-O(3)$^{\#8}$	2.010(14)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.538(8)	Li(1)-O(2)	2.137(13)
Sr(1)/Pb(1)-O(1)$^{\#4}$	2.543(6)	Li(1)-O(1)$^{\#8}$	2.164(13)
Sr(1)/Pb(1)-O(1)	2.696(7)	B(1)-O(1)	1.369(9)
Sr(1)/Pb(1)-O(3)$^{\#7}$	2.828(8)	B(1)-O(3)	1.371(10)
		B(1)-O(2)	1.379(9)
	$LiSr_{0.715}Pb_{0.285}BO_3$		
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.441(6)	Li(1)-O(3)	1.934(13)
Sr(1)/Pb(1)-O(2)	2.513(6)	Li(1)-O(2)$^{\#5}$	1.968(15)
Sr(1)/Pb(1)-O(1)$^{\#2}$	2.560(5)	Li(1)-O(3)$^{\#8}$	1.995(12)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.568(6)	Li(1)-O(1)$^{\#8}$	2.158(15)
Sr(1)/Pb(1)-O(2)$^{\#4}$	2.582(5)	Li(1)-O(2)	2.185(15)
Sr(1)/Pb(1)-O(1)	2.712(6)	B(1)-O(3)	1.354(11)
Sr(1)/Pb(1)-O(3)$^{\#7}$	2.977(9)	B(1)-O(2)	1.362(10)
		B(1)-O(1)	1.393(10)
	$LiSr_{0.680}Pb_{0.320}BO_3$		
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.411(7)	Li(1)-O(2)$^{\#5}$	1.920(17)
Sr(1)/Pb(1)-O(2)	2.503(7)	Li(1)-O(3)	1.974(19)
Sr(1)/Pb(1)-O(1)$^{\#2}$	2.543(7)	Li(1)-O(3)$^{\#8}$	1.977(16)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.603(9)	Li(1)-O(2)	2.16(2)
Sr(1)/Pb(1)-O(2)$^{\#4}$	2.612(6)	Li(1)-O(1)$^{\#8}$	2.21(2)
Sr(1)/Pb(1)-O(1)	2.726(7)	B(1)-O(3)	1.339(17)
Sr(1)/Pb(1)-O(3)$^{\#7}$	3.045(14)	B(1)-O(1)	1.368(12)
		B(1)-O(2)	1.376(14)
	$LiSr_{0.621}Pb_{0.371}BO_3$		
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.421(7)	Li(1)-O(3)	1.92(2)
Sr(1)/Pb(1)-O(2)	2.491(8)	Li(1)-O(2)$^{\#5}$	1.977(18)
Sr(1)/Pb(1)-O(1)$^{\#2}$	2.547(7)	Li(1)-O(3)$^{\#8}$	1.985(19)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.596(9)	Li(1)-O(2)	2.19(2)
Sr(1)/Pb(1)-O(2)$^{\#4}$	2.605(7)	Li(1)-O(1)$^{\#8}$	2.19(2)
Sr(1)/Pb(1)-O(1)	2.725(7)	B(1)-O(3)	1.341(14)
Sr(1)/Pb(1)-O(3)$^{\#6}$	3.062(13)	B(1)-O(1)	1.382(12)
		B(1)-O(2)	1.389(12)
	$LiSr_{0.583}Pb_{0.417}BO_3$		
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.410(8)	Li(1)-O(3)	1.933(19)
Sr(1)/Pb(1)-O(2)	2.497(7)	Li(1)-O(2)$^{\#5}$	1.96(2)
Sr(1)/Pb(1)-O(1)$^{\#2}$	2.542(7)	Li(1)-O(3)$^{\#8}$	1.963(17)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.598(8)	Li(1)-O(2)	2.17(2)
Sr(1)/Pb(1)-O(2)$^{\#4}$	2.626(8)	Li(1)-O(1)$^{\#8}$	2.219(19)
Sr(1)/Pb(1)-O(1)	2.724(7)	B(1)-O(3)	1.353(14)

Sr(1)/Pb(1)-O(3)$^{\#6}$	3.080(14)	B(1)-O(2)	1.381(14)
		B(1)-O(1)	1.381(14)
		$LiSr_{0.5}Pb_{0.5}BO_3$	
Sr(1)/Pb(1)-O(1)$^{\#1}$	2.381(6)	Li(1)-O(2)$^{\#5}$	1.934(15)
Sr(1)/Pb(1)-O(2)	2.485(6)	Li(1)-O(3)	1.946(16)
Sr(1)/Pb(1)-O(1)$^{\#2}$	2.543(6)	Li(1)-O(3)$^{\#8}$	1.972(16)
Sr(1)/Pb(1)-O(3)$^{\#3}$	2.583(8)	Li(1)-O(1)$^{\#8}$	2.166(17)
Sr(1)/Pb(1)-O(2)$^{\#4}$	2.629(6)	Li(1)-O(2)	2.205(17)
Sr(1)/Pb(1)-O(1)	2.745(7)	B(1)-O(3)	1.346(12)
Sr(1)/Pb(1)-O(3)$^{\#7}$	3.084(12)	B(1)-O(2)	1.378(10)
		B(1)-O(1)	1.391(10)

Table S2 Atom-cutting analysis and calculated birefringence at 1064nm for $LiSrBO_3$ and $LiSr_{0.5}Pb_{0.5}BO_3$

$LiSrBO_3$			$LiSr_{0.5}Pb_{0.5}BO_3$		
Species	**Δn**	**Contribution**	**Species**	**Δn**	**Contribution**
Li^+	0.0009	1.7%	Li^+	0.0016	2.5%
Sr^{2+}	0.0059	11.3%	Sr^{2+}	0.0020	3.1%
			Pb^{2+}	0.0059	9.3%
BO_3^{3-}	0.0457	87.0%	BO_3^{3-}	0.0544	85.1%
Calcd	0.0494		**Calcd**	0.0721	

Figure S1 XRD patterns of calculated and experimental for crystals $LiSr_{1-x}Pb_xBO_3$ (x=0.138, 0.285, 0.320, 0.379, 0.417, 0. 5).

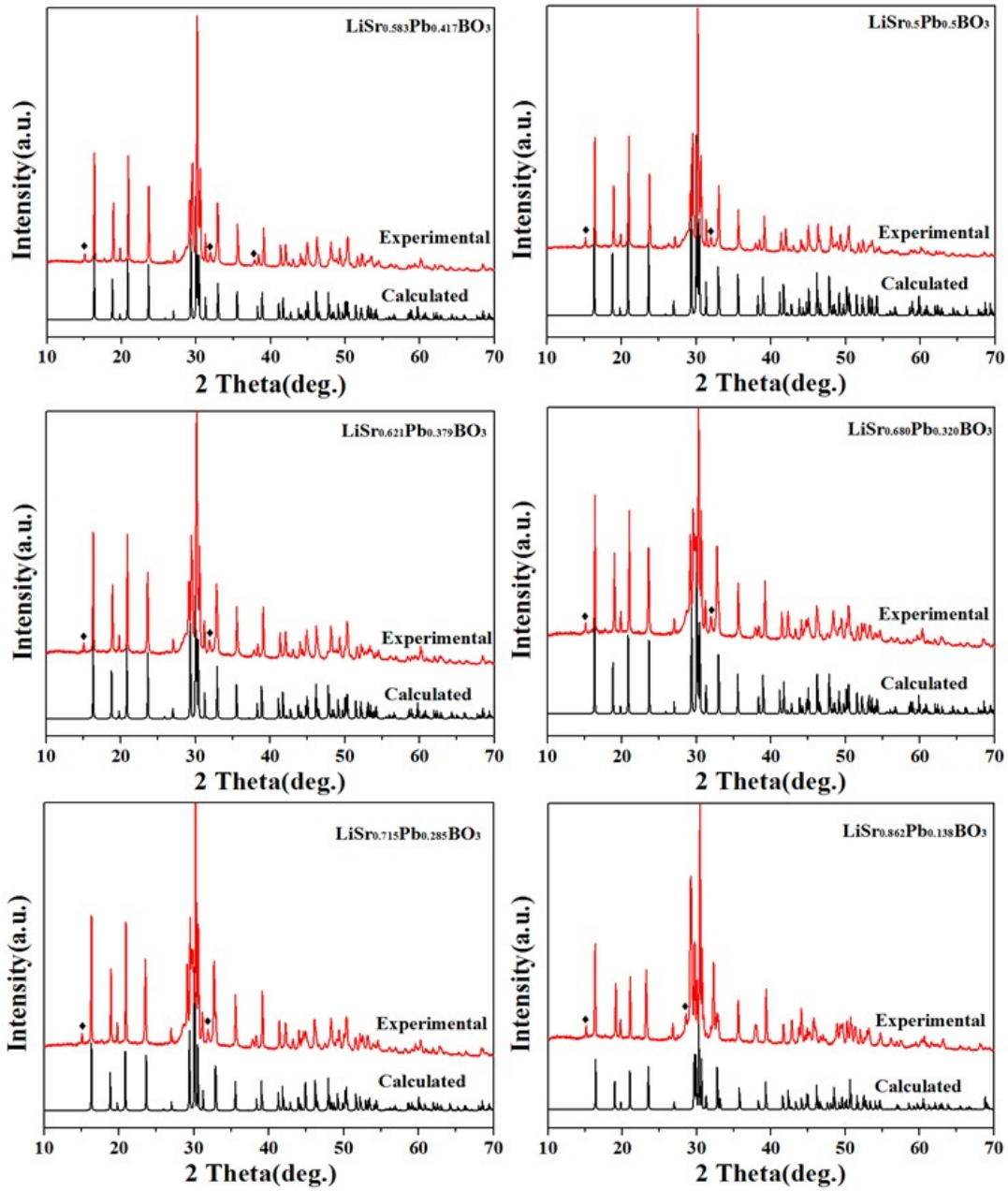

Figure S2 The calculated birefringence of $LiSrBO_3$ and $LiSr_{0.5}Pb_{0.5}BO_3$