

Electronic Supplementary Information

Structural Insights for Three Phosphates with Distinct Polyanionic Configurations

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Table S1. The final Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LiSrP_3O_9 , U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor, and the Bond Valence Sum for each atom in asymmetric unit.

Atom	x	y	z	U(eq)	BVS
Li(1)	-4630(30)	6640(30)	6700(20)	29(4)	0.92
Sr(1)	168(1)	7278(1)	6527(1)	10(1)	2.18
P(1)	4127(3)	8838(3)	2802(3)	8(1)	5.21
P(2)	2304(3)	6539(3)	10556(3)	9(1)	5.15
P(3)	-1511(3)	7871(3)	2654(3)	8(1)	5.11
O(1)	2928(8)	6397(8)	8545(8)	12(1)	2.07
O(2)	-701(8)	9432(7)	3316(8)	13(1)	2.08
O(3)	-3526(8)	8552(8)	1896(8)	14(1)	2.04
O(4)	-100(8)	7320(8)	10742(8)	10(1)	2.22
O(5)	3205(9)	8270(7)	1126(8)	13(1)	1.90
O(6)	3757(9)	7485(8)	4470(8)	14(1)	2.18
O(7)	-1659(9)	6180(8)	4016(7)	13(1)	1.98
O(8)	2582(9)	4847(8)	11879(8)	13(1)	2.07
O(9)	3495(9)	10884(8)	2960(8)	16(1)	1.97

Table S2. The final Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LiCsP_2O_6 , U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor, and the Bond Valence Sum for each atom in asymmetric unit.

Atom	x	y	z	U(eq)	BVS
Cs(1)	1359(1)	6426(1)	1223(1)	32(1)	0.95
P(1)	1014(1)	3569(1)	847(1)	20(1)	5.32
P(2)	3729(1)	8262(1)	873(1)	23(1)	5.84
O(1)	1842(2)	4126(2)	1288(2)	33(1)	2.07
O(2)	1219(2)	2395(2)	909(2)	28(1)	2.33
O(3)	711(2)	3754(2)	-171(2)	35(1)	2.01
O(4A)	4538(3)	8618(3)	1626(3)	31(1)	2.33
O(4B)	4884(4)	8704(4)	876(5)	19(2)	2.28
O(5A)	2743(4)	8456(5)	1321(3)	37(2)	1.97
O(5B)	3099(6)	9049(7)	1350(5)	24(3)	1.89
O(6A)	3948(5)	8553(5)	-137(3)	44(2)	2.04
O(6B)	3539(7)	7966(7)	-127(5)	24(3)	2.06
Li(1)	3272(5)	4040(5)	1250(4)	33(2)	1.09

Table S3. The final Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{K}_2\text{CsP}_4\text{O}_{12}$, U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor, and the Bond Valence Sum for each atom in asymmetric unit.

Atom	x	y	z	U(eq)	BVS
Sr(1)	5000	10000	2500	10(1)	2.26
K(2)	5000	5000	1732(1)	24(1)	1.09
P(3)	8417(1)	12187(1)	339(1)	10(1)	5.11
O(1)	3855(3)	11926(3)	414(2)	16(1)	1.97
O(3)	6951(3)	4469(3)	4353(2)	13(1)	2.19
O(2)	7528(3)	11881(3)	1626(2)	15(1)	2.09

Table S4. Selected bond distances (Å) and angles (deg) for LiSrP₃O₉.

Li(1)-O(1)#1	1.963(18)	O(2)#3-Sr(1)-O(8)#2	134.92(19)
Li(1)-O(8)#2	1.990(18)	O(1)-Sr(1)-O(8)#2	102.58(19)
Li(1)-O(9)#3	2.086(18)	O(7)#4-Sr(1)-O(8)#2	73.08(19)
Li(1)-O(6)#1	2.118(17)	O(9)#3-Sr(1)-O(8)#2	66.5(2)
Li(1)-O(7)	2.570(19)	O(2)#3-Sr(1)-O(6)	76.89(18)
Sr(1)-O(2)#3	2.453(6)	O(1)-Sr(1)-O(6)	70.3(2)
Sr(1)-O(1)	2.552(6)	O(7)#4-Sr(1)-O(6)	74.80(18)
Sr(1)-O(7)#4	2.576(6)	O(9)#3-Sr(1)-O(6)	141.06(19)
Sr(1)-O(9)#3	2.614(7)	O(8)#2-Sr(1)-O(6)	147.79(18)
Sr(1)-O(8)#2	2.615(6)	O(2)#3-Sr(1)-O(7)	123.95(18)
Sr(1)-O(6)	2.642(6)	O(1)-Sr(1)-O(7)	146.07(18)
Sr(1)-O(7)	2.642(6)	O(7)#4-Sr(1)-O(7)	72.3(2)
Sr(1)-O(2)	2.781(6)	O(9)#3-Sr(1)-O(7)	74.85(19)
P(1)-O(9)	1.474(6)	O(8)#2-Sr(1)-O(7)	69.83(18)
P(1)-O(6)	1.487(6)	O(6)-Sr(1)-O(7)	98.1(2)
P(1)-O(5)	1.592(6)	O(2)#3-Sr(1)-O(2)	70.6(2)
P(1)-O(3)#5	1.604(6)	O(1)-Sr(1)-O(2)	142.31(17)
P(2)-O(1)	1.477(6)	O(7)#4-Sr(1)-O(2)	113.16(17)
P(2)-O(8)	1.479(6)	O(9)#3-Sr(1)-O(2)	68.83(18)
P(2)-O(5)#6	1.586(5)	O(8)#2-Sr(1)-O(2)	114.98(17)
P(2)-O(4)	1.627(6)	O(6)-Sr(1)-O(2)	76.01(18)
P(3)-O(2)	1.478(6)	O(7)-Sr(1)-O(2)	54.46(17)
P(3)-O(7)	1.488(6)	O(2)#3-Sr(1)-O(4)	80.07(17)
P(3)-O(3)	1.555(6)	O(1)-Sr(1)-O(4)	50.12(17)
P(3)-O(4)#7	1.608(6)	O(7)#4-Sr(1)-O(4)	102.46(16)
O(1)-Li(1)#5	1.963(18)	O(9)#3-Sr(1)-O(4)	85.01(17)
O(2)-Sr(1)#3	2.453(6)	O(8)#2-Sr(1)-O(4)	72.68(16)
O(3)-P(1)#1	1.604(6)	O(6)-Sr(1)-O(4)	117.13(16)
O(4)-P(3)#6	1.608(6)	O(7)-Sr(1)-O(4)	142.02(16)
O(5)-P(2)#7	1.586(5)	O(2)-Sr(1)-O(4)	144.31(16)
O(6)-Li(1)#5	2.118(17)	O(6)-P(1)-O(5)	111.4(3)
O(7)-Sr(1)#4	2.576(6)	O(9)-P(1)-O(3)#5	107.9(3)
O(8)-Li(1)#2	1.990(18)	O(6)-P(1)-O(3)#5	110.2(3)
O(8)-Sr(1)#2	2.615(6)	O(5)-P(1)-O(3)#5	98.4(3)
O(9)-Li(1)#3	2.086(18)	O(8)-P(2)-O(5)#6	111.4(3)
O(9)-Sr(1)#3	2.614(7)	O(1)-P(2)-O(4)	103.1(3)
O(1)#1-Li(1)-O(8)#2	99.1(8)	O(8)-P(2)-O(4)	108.7(3)
O(1)#1-Li(1)-O(9)#3	108.9(10)	O(5)#6-P(2)-O(4)	102.3(3)
O(8)#2-Li(1)-O(9)#3	89.3(7)	O(1)-P(2)-O(8)	120.5(3)
O(1)#1-Li(1)-O(6)#1	94.2(7)	O(1)-P(2)-O(5)#6	108.8(3)
O(8)#2-Li(1)-O(6)#1	158.2(11)	O(2)-P(3)-O(7)	113.8(3)
O(9)#3-Li(1)-O(6)#1	102.7(7)	O(2)-P(3)-O(3)	112.4(3)
O(1)#1-Li(1)-O(7)	165.1(10)	O(7)-P(3)-O(3)	112.3(3)

O(8)#2-Li(1)-O(7)	81.5(7)	O(2)-P(3)-O(4)#7	107.8(3)
O(9)#3-Li(1)-O(7)	86.0(6)	O(7)-P(3)-O(4)#7	111.0(3)
O(6)#1-Li(1)-O(7)	81.3(6)	O(3)-P(3)-O(4)#7	98.4(3)
O(2)#3-Sr(1)-O(1)	85.50(18)	O(2)#3-Sr(1)-O(9)#3	76.12(19)
O(2)#3-Sr(1)-O(7)#4	149.2(2)	O(1)-Sr(1)-O(9)#3	134.04(19)
O(1)-Sr(1)-O(7)#4	73.90(17)	O(7)#4-Sr(1)-O(9)#3	134.48(18)

Symmetry transformations used to generate equivalent atoms:

#1 $x-1, y, z$ #2 $-x, -y+1, -z+2$ #3 $-x, -y+2, -z+1$ #4 $-x, -y+1, -z+1$
#5 $x+1, y, z$ #6 $x, y, z+1$ #7 $x, y, z-1$

Table S5. Selected bond distances (Å) and angles (deg) for LiCsP₂O₆.

Cs(1)-O(6B)#1	2.945(9)	O(6B)#1-Cs(1)-O(5B)#4	68.2(2)
Cs(1)-O(5B)#2	3.006(11)	O(5B)#2-Cs(1)-O(5B)#4	76.66(16)
Cs(1)-O(3)#3	3.125(3)	O(3)#3-Cs(1)-O(5B)#4	127.81(15)
Cs(1)-O(1)	3.139(3)	O(1)-Cs(1)-O(5B)#4	75.52(16)
Cs(1)-O(4A)#4	3.175(5)	O(4A)#4-Cs(1)-O(5B)#4	35.56(14)
Cs(1)-O(2)#5	3.192(3)	O(2)#5-Cs(1)-O(5B)#4	164.34(18)
Cs(1)-O(6A)#6	3.263(6)	O(6A)#6-Cs(1)-O(5B)#4	74.19(18)
Cs(1)-O(5A)	3.282(8)	O(5A)-Cs(1)-O(5B)#4	89.7(2)
Cs(1)-O(4B)#6	3.349(7)	O(4B)#6-Cs(1)-O(5B)#4	41.97(17)
Cs(1)-O(5B)#4	3.453(7)	O(6B)#1-Cs(1)-O(4A)#2	155.51(16)
Cs(1)-O(4A)#2	3.498(4)	O(5B)#2-Cs(1)-O(4A)#2	35.58(14)
Cs(1)-O(1)#7	3.499(4)	O(3)#3-Cs(1)-O(4A)#2	143.81(9)
P(1)-O(1)	1.462(3)	O(1)-Cs(1)-O(4A)#2	91.98(8)
P(1)-O(3)	1.469(3)	O(4A)#4-Cs(1)-O(4A)#2	119.58(11)
P(1)-O(2)	1.593(3)	O(2)#5-Cs(1)-O(4A)#2	80.66(8)
P(1)-O(2)#8	1.596(3)	O(6A)#6-Cs(1)-O(4A)#2	88.99(13)
P(2)-O(6B)	1.444(7)	O(5A)-Cs(1)-O(4A)#2	43.16(10)
P(2)-O(6A)	1.463(5)	O(4B)#6-Cs(1)-O(4A)#2	93.90(13)
P(2)-O(5A)	1.474(5)	O(5B)#4-Cs(1)-O(4A)#2	88.38(16)
P(2)-O(5B)	1.495(7)	O(6B)#1-Cs(1)-O(1)#7	122.69(14)
P(2)-O(4B)#2	1.561(6)	O(5B)#2-Cs(1)-O(1)#7	76.49(13)
P(2)-O(4A)	1.566(4)	O(3)#3-Cs(1)-O(1)#7	68.29(7)
P(2)-O(4A)#2	1.646(4)	O(1)-Cs(1)-O(1)#7	73.70(6)
P(2)-O(4B)	1.651(6)	O(4A)#4-Cs(1)-O(1)#7	155.93(9)
O(1)-Cs(1)#1	3.499(4)	O(2)#5-Cs(1)-O(1)#7	42.06(7)
O(2)-P(1)#11	1.596(3)	O(6A)#6-Cs(1)-O(1)#7	136.19(10)
O(2)-Cs(1)#9	3.192(3)	O(5A)-Cs(1)-O(1)#7	102.91(9)
O(3)-Li#7	1.948(7)	O(4B)#6-Cs(1)-O(1)#7	168.58(11)
O(3)-Cs(1)#3	3.125(3)	O(5B)#4-Cs(1)-O(1)#7	146.90(13)
O(3)-Cs(1)#9	3.532(3)	O(4A)#2-Cs(1)-O(1)#7	80.86(8)
O(4A)-O(4B)	1.129(7)	O(1)-P(1)-O(3)	120.81(17)
O(4A)-P(2)#10	1.646(4)	O(1)-P(1)-O(2)	110.44(15)
O(4A)-Cs(1)#4	3.175(5)	O(3)-P(1)-O(2)	105.25(15)
O(4A)-Cs(1)#10	3.498(4)	O(1)-P(1)-O(2)#8	104.43(15)
O(4B)-P(2)#10	1.561(6)	O(3)-P(1)-O(2)#8	111.85(16)
O(4B)-Cs(1)#12	3.349(7)	O(2)-P(1)-O(2)#8	102.70(17)
O(4B)-Cs(1)#10	3.538(6)	O(6B)-P(2)-O(6A)	38.3(3)
O(5A)-O(5B)	0.923(7)	O(6B)-P(2)-O(5A)	106.5(4)
O(5A)-Li#10	1.911(8)	O(6A)-P(2)-O(5A)	121.5(3)
O(5A)-Cs(1)#4	3.567(5)	O(6B)-P(2)-O(5B)	120.4(4)
O(5B)-Li#10	2.099(10)	O(6A)-P(2)-O(5B)	109.7(4)
O(5B)-Cs(1)#10	3.006(10)	O(5A)-P(2)-O(5B)	36.2(3)
O(5B)-Cs(1)#4	3.453(7)	O(6B)-P(2)-O(4B)#2	115.2(5)

O(6A)-O(6B)	0.954(8)	O(6A)-P(2)-O(4B)#2	143.9(3)
O(6A)-Li#5	1.884(8)	O(5A)-P(2)-O(4B)#2	84.8(3)
O(6A)-Cs(1)#12	3.263(6)	O(5B)-P(2)-O(4B)#2	105.8(4)
O(6A)-Cs(1)#7	3.577(7)	O(6B)-P(2)-O(4A)	145.6(4)
O(6B)-Li#5	2.131(11)	O(6A)-P(2)-O(4A)	113.7(3)
O(6B)-Cs(1)#7	2.945(8)	O(5A)-P(2)-O(4A)	106.9(3)
Li-O(6A)#9	1.884(8)	O(5B)-P(2)-O(4A)	83.6(4)
Li-O(5A)#2	1.911(8)	O(4B)#2-P(2)-O(4A)	75.9(3)
Li-O(3)#1	1.948(7)	O(6B)-P(2)-O(4A)#2	75.6(4)
Li-O(5B)#2	2.099(10)	O(6A)-P(2)-O(4A)#2	103.9(3)
Li-O(6B)#9	2.131(11)	O(5A)-P(2)-O(4A)#2	106.5(3)
O(5A)-Cs(1)-O(4B)#6	66.89(13)	O(5B)-P(2)-O(4A)#2	140.0(4)
O(6B)#1-Cs(1)-O(5B)#2	136.2(2)	O(4B)#2-P(2)-O(4A)#2	41.1(3)
O(6B)#1-Cs(1)-O(3)#3	60.01(17)	O(4A)-P(2)-O(4A)#2	102.4(3)
O(5B)#2-Cs(1)-O(3)#3	141.13(13)	O(6B)-P(2)-O(4B)	105.3(5)
O(6B)#1-Cs(1)-O(1)	89.0(2)	O(6A)-P(2)-O(4B)	73.8(4)
O(5B)#2-Cs(1)-O(1)	56.65(13)	O(5A)-P(2)-O(4B)	140.3(4)
O(3)#3-Cs(1)-O(1)	96.86(7)	O(5B)-P(2)-O(4B)	105.9(5)
O(6B)#1-Cs(1)-O(4A)#4	35.94(16)	O(4B)#2-P(2)-O(4B)	102.3(4)
O(5B)#2-Cs(1)-O(4A)#4	111.98(15)	O(4A)-P(2)-O(4B)	41.0(3)
O(3)#3-Cs(1)-O(4A)#4	95.20(9)	O(4A)#2-P(2)-O(4B)	103.8(3)
O(1)-Cs(1)-O(4A)#4	91.88(9)	O(5A)#2-Li-O(6B)#9	116.0(4)
O(6B)#1-Cs(1)-O(2)#5	120.62(19)	O(1)-Li-O(6B)#9	103.1(4)
O(5B)#2-Cs(1)-O(2)#5	100.00(14)	O(3)#1-Li-O(6B)#9	96.2(4)
O(3)#3-Cs(1)-O(2)#5	63.87(7)	O(5B)#2-Li-O(6B)#9	126.9(4)
O(1)-Cs(1)-O(2)#5	115.75(7)	O(6A)#6-Cs(1)-O(4B)#6	32.93(14)
O(4A)#4-Cs(1)-O(2)#5	146.11(9)	O(6A)#9-Li-O(5A)#2	89.5(4)
O(6B)#1-Cs(1)-O(6A)#6	78.12(15)	O(6A)#9-Li-O(1)	121.3(4)
O(5B)#2-Cs(1)-O(6A)#6	116.87(18)	O(5A)#2-Li-O(1)	119.3(5)
O(3)#3-Cs(1)-O(6A)#6	100.13(14)	O(6A)#9-Li-O(3)#1	105.0(4)
O(1)-Cs(1)-O(6A)#6	149.65(11)	O(5A)#2-Li-O(3)#1	109.9(4)
O(4A)#4-Cs(1)-O(6A)#6	61.78(11)	O(1)-Li-O(3)#1	109.7(3)
O(2)#5-Cs(1)-O(6A)#6	94.34(11)	O(6A)#9-Li-O(5B)#2	103.6(4)
O(6B)#1-Cs(1)-O(5A)	126.07(17)	O(5A)#2-Li-O(5B)#2	26.1(2)
O(5B)#2-Cs(1)-O(5A)	77.38(14)	O(1)-Li-O(5B)#2	93.2(4)
O(3)#3-Cs(1)-O(5A)	125.49(9)	O(3)#1-Li-O(5B)#2	125.1(4)
O(1)-Cs(1)-O(5A)	133.67(9)	O(6A)#9-Li-O(6B)#9	26.6(2)
O(4A)#4-Cs(1)-O(5A)	100.97(11)	O(5B)#2-Cs(1)-O(4B)#6	105.10(16)
O(2)#5-Cs(1)-O(5A)	74.68(9)	O(3)#3-Cs(1)-O(4B)#6	112.71(12)
O(6A)#6-Cs(1)-O(5A)	48.18(13)	O(1)-Cs(1)-O(4B)#6	116.84(12)
O(6B)#1-Cs(1)-O(4B)#6	64.12(17)	O(4A)#4-Cs(1)-O(4B)#6	34.16(13)
O(2)#5-Cs(1)-O(4B)#6	127.26(12)		

Symmetry transformations used to generate equivalent atoms:

#1 -y+3/4,x+1/4,z+1/4 #2 -y+5/4,x+1/4,-z+1/4 #3 -x,-y+1,-z

#4 $-x+1/2, -y+3/2, -z+1/2$ #5 $x, y+1/2, -z$ #6 $y-3/4, -x+5/4, z+1/4$
#7 $y-1/4, -x+3/4, z-1/4$ #8 $-y+1/4, x+1/4, -z+1/4$ #9 $x, y-1/2, -z$
#10 $y-1/4, -x+5/4, -z+1/4$ #11 $y-1/4, -x+1/4, -z+1/4$ #12 $-y+5/4, x+3/4, z-1/4$

Table S6. Selected bond distances (Å) and angles (deg) for K₂SrP₄O₁₂.

Sr(1)-O(2)	2.503(2)	O(1)#4-K(2)-O(2)#2	164.14(6)
Sr(1)-O(2)#1	2.503(2)	O(1)#3-K(2)-O(2)#2	66.52(8)
Sr(1)-O(2)#2	2.503(2)	O(2)#5-K(2)-O(2)#2	108.34(11)
Sr(1)-O(2)#3	2.503(2)	O(1)#4-K(2)-O(2)#3	115.34(7)
Sr(1)-O(1)	2.693(3)	O(1)#3-K(2)-O(2)#3	62.43(6)
Sr(1)-O(1)#3	2.693(3)	O(2)#5-K(2)-O(2)#3	102.32(8)
Sr(1)-O(1)#1	2.693(3)	O(2)#2-K(2)-O(2)#3	80.15(8)
Sr(1)-O(1)#2	2.693(3)	O(1)#4-K(2)-O(2)#4	62.43(6)
K(2)-O(1)#4	2.780(3)	O(1)#3-K(2)-O(2)#4	115.34(7)
K(2)-O(1)#3	2.780(3)	O(2)#5-K(2)-O(2)#4	80.15(8)
K(2)-O(2)#5	2.846(3)	O(2)#2-K(2)-O(2)#4	102.32(8)
K(2)-O(2)#2	2.846(3)	O(2)#3-K(2)-O(2)#4	175.85(9)
K(2)-O(2)#3	2.985(3)	O(1)#4-K(2)-O(3)#6	112.34(7)
K(2)-O(2)#4	2.985(3)	O(1)#3-K(2)-O(3)#6	117.26(7)
K(2)-O(3)#6	3.055(3)	O(2)#5-K(2)-O(3)#6	48.76(6)
K(2)-O(3)	3.055(3)	O(2)#2-K(2)-O(3)#6	68.88(7)
K(2)-O(1)#7	3.269(3)	O(2)#3-K(2)-O(3)#6	68.45(6)
K(2)-O(1)#8	3.269(3)	O(2)#4-K(2)-O(3)#6	115.49(7)
P(3)-O(1)#10	1.478(2)	O(1)#4-K(2)-O(3)	117.26(7)
P(3)-O(2)	1.481(2)	O(1)#3-K(2)-O(3)	112.34(7)
P(3)-O(3)#11	1.609(2)	O(2)#5-K(2)-O(3)	68.88(7)
P(3)-O(3)#1	1.612(2)	O(2)#2-K(2)-O(3)	48.76(6)
O(1)-P(3)#15	1.478(2)	O(2)#3-K(2)-O(3)	115.49(7)
O(1)-K(2)#12	2.780(3)	O(2)#4-K(2)-O(3)	68.45(6)
O(1)-K(2)#16	3.269(3)	O(3)#6-K(2)-O(3)	58.91(9)
O(3)-P(3)#17	1.609(2)	O(1)#4-K(2)-O(1)#7	71.29(4)
O(3)-P(3)#2	1.612(2)	O(1)#3-K(2)-O(1)#7	71.29(4)
O(2)-K(2)#13	2.846(3)	O(2)#5-K(2)-O(1)#7	102.42(7)
O(2)-K(2)#12	2.985(3)	O(2)#2-K(2)-O(1)#7	124.42(6)
O(2)-Sr(1)-O(2)#1	97.22(4)	O(2)#3-K(2)-O(1)#7	48.26(6)
O(2)-Sr(1)-O(2)#2	97.22(4)	O(2)#4-K(2)-O(1)#7	128.13(7)
O(2)#1-Sr(1)-O(2)#2	138.48(11)	O(3)#6-K(2)-O(1)#7	102.43(8)
O(2)-Sr(1)-O(2)#3	138.48(11)	O(3)-K(2)-O(1)#7	160.98(6)
O(2)#1-Sr(1)-O(2)#3	97.22(4)	O(1)#4-K(2)-O(1)#8	71.29(4)
O(2)#2-Sr(1)-O(2)#3	97.22(4)	O(1)#3-K(2)-O(1)#8	71.29(4)
O(2)-Sr(1)-O(1)	70.23(7)	O(2)#5-K(2)-O(1)#8	124.42(6)
O(2)#1-Sr(1)-O(1)	72.77(8)	O(2)#2-K(2)-O(1)#8	102.42(7)
O(2)#2-Sr(1)-O(1)	148.59(7)	O(2)#3-K(2)-O(1)#8	128.13(7)
O(2)#3-Sr(1)-O(1)	77.35(7)	O(2)#4-K(2)-O(1)#8	48.26(6)
O(2)-Sr(1)-O(1)#3	77.35(7)	O(3)#6-K(2)-O(1)#8	160.98(6)
O(2)#1-Sr(1)-O(1)#3	148.59(7)	O(3)-K(2)-O(1)#8	102.43(8)
O(2)#2-Sr(1)-O(1)#3	72.77(8)	O(1)#7-K(2)-O(1)#8	96.41(10)
O(2)#3-Sr(1)-O(1)#3	70.23(7)	O(1)#10-P(3)-O(2)	120.54(14)

O(1)-Sr(1)-O(1)#3	76.35(11)	O(1)#10-P(3)-O(3)#11	106.85(13)
O(2)-Sr(1)-O(1)#1	148.59(7)	O(2)-P(3)-O(3)#11	110.82(13)
O(2)#1-Sr(1)-O(1)#1	70.23(7)	O(1)#10-P(3)-O(3)#1	111.06(13)
O(2)#2-Sr(1)-O(1)#1	77.35(7)	O(2)-P(3)-O(3)#1	104.31(13)
O(2)#3-Sr(1)-O(1)#1	72.77(8)	O(3)#11-P(3)-O(3)#1	101.69(15)
O(1)-Sr(1)-O(1)#1	128.17(7)	O(1)#1-Sr(1)-O(1)#2	76.35(11)
O(1)#3-Sr(1)-O(1)#1	128.17(7)	O(1)#4-K(2)-O(1)#3	122.47(12)
O(2)-Sr(1)-O(1)#2	72.77(8)	O(1)#4-K(2)-O(2)#5	66.52(8)
O(2)#1-Sr(1)-O(1)#2	77.35(7)	O(1)#3-K(2)-O(2)#5	164.14(6)
O(2)#2-Sr(1)-O(1)#2	70.23(7)	O(1)#3-Sr(1)-O(1)#2	128.17(7)
O(2)#3-Sr(1)-O(1)#2	148.59(7)	O(1)-Sr(1)-O(1)#2	128.17(7)

Symmetry transformations used to generate equivalent atoms:

#1 $-y+3/2, x+1/2, -z+1/2$ #2 $y-1/2, -x+3/2, -z+1/2$ #3 $-x+1, -y+2, z$
#4 $x, y-1, z$ #5 $-y+3/2, x-1/2, -z+1/2$ #6 $-x+1, -y+1, z$ #7 $y-1, -x+1, -z$
#8 $-y+2, x, -z$ #9 $y, -x+1, -z$ #10 $-y+2, x+1, -z$ #11 $-x+3/2, -y+3/2, z-1/2$
#12 $x, y+1, z$ #13 $y+1/2, -x+3/2, -z+1/2$
#14 $x+1/2, y+1/2, z-1/2$ #15 $y-1, -x+2, -z$

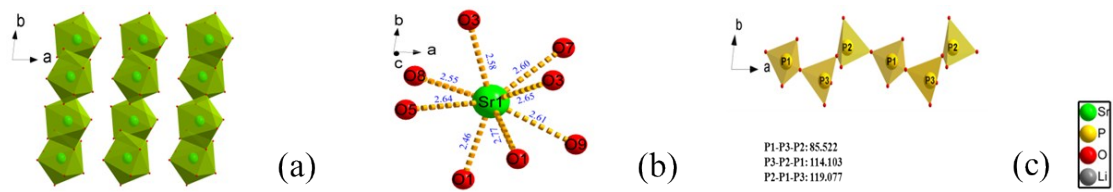


Figure S1. (a) The arrangement of the SrO_8 groups; (b) Coordination environment of the Sr atom; (c) The 1D infinite $(\text{PO}_3)_\infty$ chain of LiSrP_3O_9 .

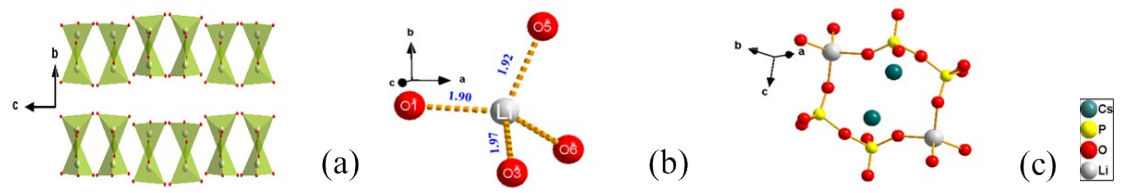


Figure S2. (a) The arrangement of the LiO₄ groups; (b) Coordination environment of the Li atom; (c) The Cs atom filled in the 3D network.

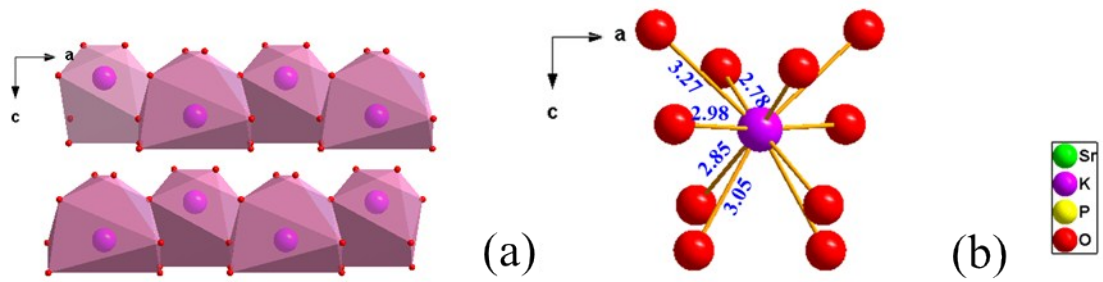


Figure S3. (a) The arrangement of the KO_{10} groups; (b) Coordination environment of the K atom.

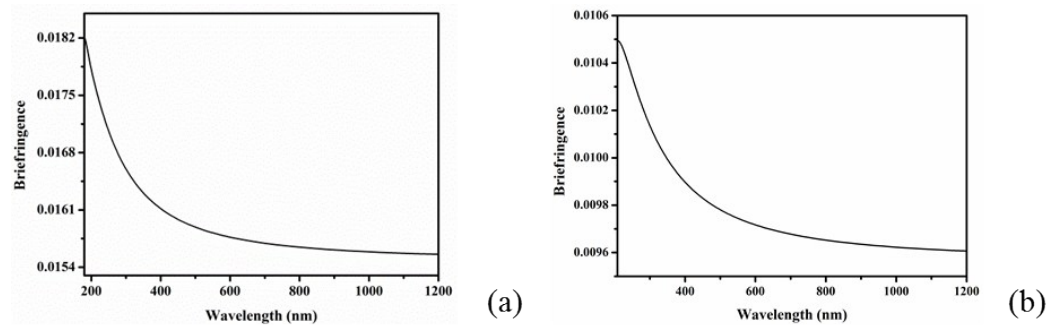


Figure S4. The frequency-dependent birefringence of LiSrP_3O_9 (a) and $\text{K}_2\text{Sr}_4\text{O}_{12}$ (b)