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# $LiSrSbS_3$: Parallel configurations of lone pair electrons inducing a large birefringence

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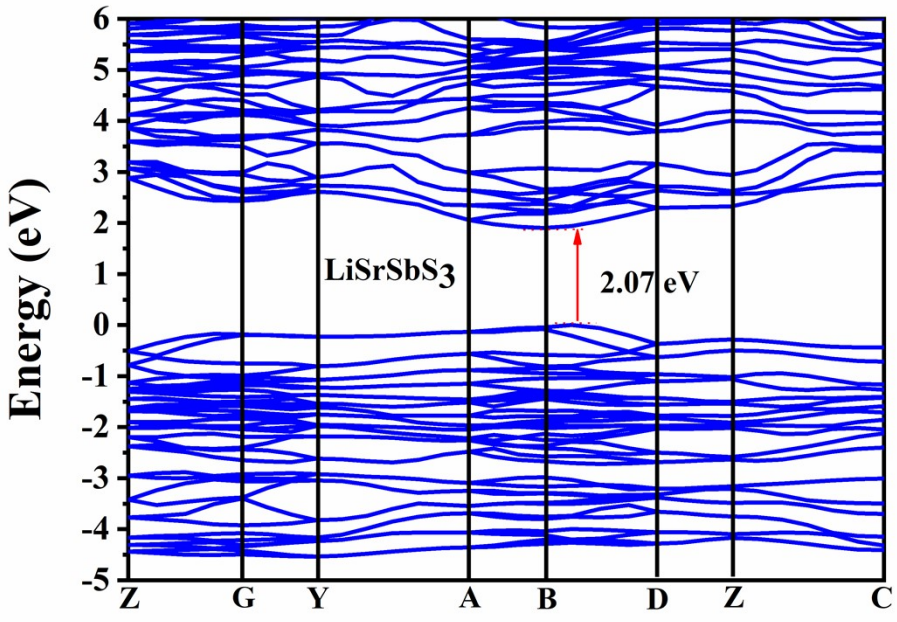


**Figure S1.** Band structure for $LiSrSbS_3$.

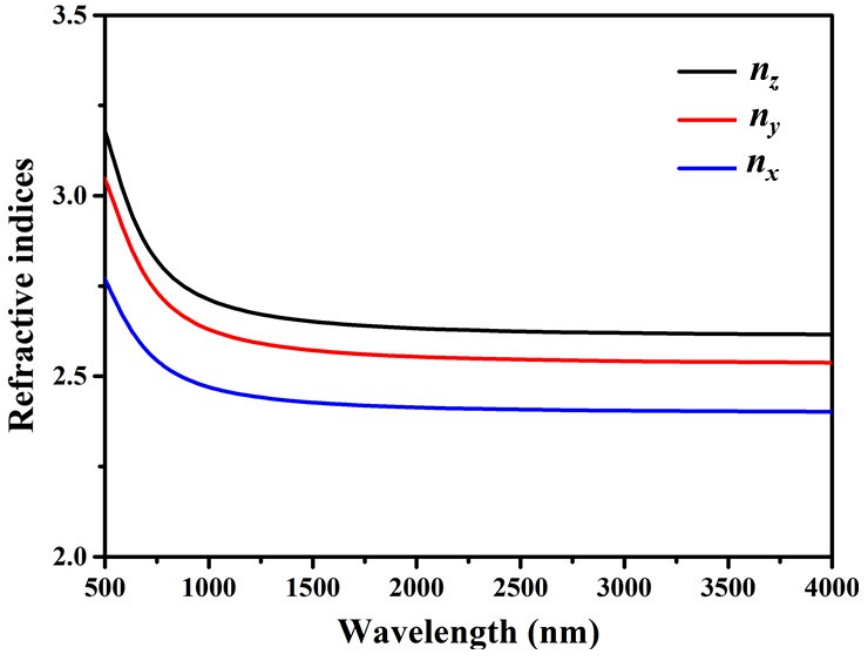


**Figure S2.** Calculated refractive indices of $LiSrSbS_3$.

**Table S1** Atomic coordinates (×$10^4$) and equivalent isotropic displacement parameters (Å$^2$×$10^3$) for $LiSrSbS_3$.

| atom | x | y | z | U(eq)[a] |
|---|---|---|---|---|
| Sb(1) | 7347(1) | 9089(1) | 1509(1) | 14(1) |
| Sr(1) | 7548(1) | 5769(1) | 1530(1) | 16(1) |
| S(1) | 3310(2) | 8799(1) | 1362(2) | 19(1) |
| S(2) | 8126(3) | 7713(1) | 3670(2) | 20(1) |
| S(3) | 7418(2) | 10666(1) | 3455(2) | 15(1) |
| Li(1) | 2535(17) | 7363(9) | 3642(15) | 31(3) |

[a]U(eq) is defined as one-third of the trace of the orthogonalized $U_{ij}$ tensor.

**Table S2** Bond lengths [Å] and angles [deg.] for $LiSrSbS_3$.

| | | | |
|---|---|---|---|
| Li(1)-S(1)#4 | 2.629(11) | S(1)-Li(1)-S(1)#4 | 157.0(5) |
| Li(1)-S(2)#8 | 2.650(10) | S(1)-Li(1)-S(2)#8 | 94.2(3) |
| Li(1)-S(3)#5 | 2.673(12) | S(1)#4-Li(1)-S(2)#8 | 104.5(3) |
| Li(1)-S(1) | 2.576(11) | S(1)-Li(1)-S(3)#5 | 95.6(4) |
| Sr(1)-S(3)#5 | 2.948(3) | S(1)#4-Li(1)-S(3)#5 | 94.8(3) |
| Sr(1)-S(2) | 2.956(2) | S(2)#8-Li(1)-S(3)#5 | 98.4(4) |
| Sr(1)-S(2)#2 | 2.964(2) | S(1)-Sb(1)-S(2) | 96.55(5) |
| Sr(1)-S(3)#6 | 2.988(3) | S(1)-Sb(1)-S(3) | 99.13(5) |
| Sr(1)-S(1)#5 | 2.994(2) | S(2)-Sb(1)-S(3) | 95.92(8) |
| Sr(1)-S(3)#2 | 3.016(2) | S(3)#5-Sr(1)-S(2) | 98.36(4) |
| Sb(1)-S(1) | 2.423(3) | S(3)#5-Sr(1)-S(2)#2 | 98.62(4) |
| Sb(1)-S(2) | 2.454(2) | S(2)-Sr(1)-S(2)#2 | 85.14(7) |
| Sb(1)-S(3) | 2.484(2) | S(3)#5-Sr(1)-S(3)#6 | 175.08(5) |
| | | | |
| S(2)-Sr(1)-S(3)#6 | 85.38(4) | | |
| S(2)#2-Sr(1)-S(3)#6 | 84.84(4) | | |
| S(3)#5-Sr(1)-S(1)#5 | 77.89(4) | | |
| S(2)-Sr(1)-S(1)#5 | 110.83(8) | | |
| S(2)#2-Sr(1)-S(1)#5 | 163.93(4) | | |
| S(3)#6-Sr(1)-S(1)#5 | 97.82(4) | | |
| S(3)#5-Sr(1)-S(3)#2 | 87.53(4) | | |
| S(2)-Sr(1)-S(3)#2 | 160.57(4) | | |
| S(2)#2-Sr(1)-S(3)#2 | 75.65(8) | | |
| S(3)#6-Sr(1)-S(3)#2 | 89.96(4) | | |
| S(1)#5-Sr(1)-S(3)#2 | 88.48(8) | | |

Symmetry transformations used to generate equivalent atoms:

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

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

#7 x+1, y, z #8 x-1, y, z

**Table S3** Anisotropic displacement parameters ($Å^2 \times 10^3$) for $LiSrSbS_3$.

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Sb(1) | 16(1) | 12(1) | 14(1) | 0(1) | 0(1) | 0(1) |
| Sr(1) | 16(1) | 15(1) | 17(1) | 0(1) | 0(1) | -2(1) |
| S(1) | 17(1) | 17(1) | 22(1) | -4(1) | -3(1) | -2(1) |
| S(2) | 32(1) | 13(1) | 15(1) | -1(1) | -1(1) | 3(1) |
| S(3) | 16(1) | 11(1) | 17(1) | -1(1) | -2(1) | -2(1) |
| Li(1) | 22(6) | 37(6) | 35(6) | 8(4) | 14(5) | 9(4) |