## **Electronic supplementary information**

## Lone Pair Effects on Ternary Infrared Nonlinear Optical Materials

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Fig. S1 Crystal structures of the  $K_3AsS_4$  (a),  $Li_3AsS_3$  (b),  $Pb_9As_4S_{15}$  (c) and  $Ag_3AsS_3$  (d)

Fig. S2 SHG density of  $K_3AsS_4\left(a\right)$  (b) and  $Pb_9As_4S_{15}\left(c\right)$  (d).

Fig. S3 Crystal structures of the  $Li_3SbS_3$  (a),  $AgSbS_2$  (b) and  $Ag_3SbS_3$  (c) (the yellow and red balls represent S and Sb atoms, respectively)







Fig. S1 Crystal structures of the  $K_3AsS_4$  (a),  $Li_3AsS_3$  (b),  $Pb_9As_4S_{15}$  (c) and  $Ag_3AsS_3$  (d)



Fig. S2 SHG density of K3AsS4 (a) (b) and Pb9As4S15 (c) (d).



Fig. S3 Crystal structures of the  $\rm Li_3SbS_3$  (a),  $\rm AgSbS_2$  (b) and  $\rm Ag_3SbS_3$  (c)