Electronic supplementary information

Lone Pair Effects on Ternary Infrared Nonlinear Optical Materials

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Fig. S1 Crystal structures of the K$_3$AsS$_4$ (a), Li$_3$AsS$_3$ (b), Pb$_9$As$_4$S$_{15}$ (c) and Ag$_3$AsS$_3$ (d)

Fig. S2 SHG density of K$_3$AsS$_4$ (a) (b) and Pb$_9$As$_4$S$_{15}$ (c) (d).

Fig. S3 Crystal structures of the Li$_3$SbS$_4$ (a), AgSbS$_3$ (b) and Ag$_3$SbS$_3$ (c) (the yellow and red balls represent S and Sb atoms, respectively)
Fig. S1 Crystal structures of the K$_3$AsS$_4$ (a), Li$_3$AsS$_3$ (b), Pb$_9$As$_4$S$_{15}$ (c) and Ag$_3$AsS$_3$ (d).

Fig. S2 SHG density of K$_3$AsS$_4$ (a) (b) and Pb$_9$As$_4$S$_{15}$ (c) (d).
Fig. S3 Crystal structures of the Li$_2$SbS$_3$ (a), AgSbS$_2$ (b) and Ag$_3$SbS$_3$ (c)