Supplementary Material (ESI) for Dalton Transactions

Syntheses, crystal structures and characterizations of two new quaternary thioborates: $PbMBS_4$ (M = Sb, Bi)†

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Electronic Supplementary Information

Table S1 The definitions and related state energies (eV) of the special k-points for $PbSbBS_4$.

k-point	H-VB[a]	L-CB[b]
G(0, 0, 0)	–0.35784	2.023093
Z(0, 0, 0.5)	–0.36782	2.329496
Y(0, 0.5, 0)	–0.16087	2.26089
A(-0.5, 0.5, 0)	–0.07326	2.162252
B(-0.5, 0, 0.0)	–0.0129	2.161991
D(-0.5, 0, 0.5)	–0.16367	2.094257
E(-0.5, 0.5, 0.5)	–0.09163	2.200215
C(0, 0.5, 0.5)	–0.07457	2.208432

[a]H-VB, the highest valence band; [b]L-CB, the lowest conduction band.

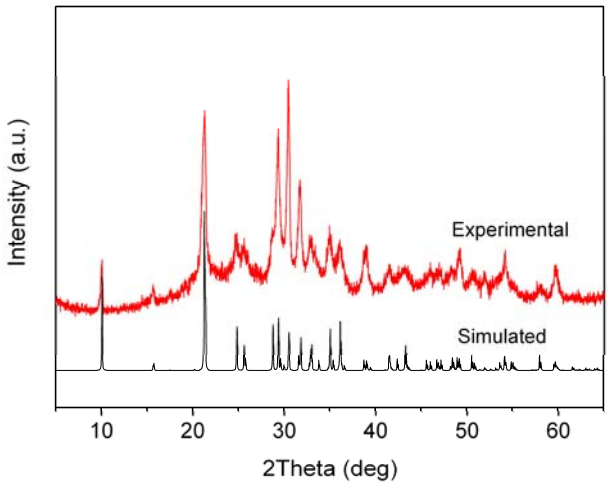

Fig. S1 X-ray powder diffraction pattern for compound $PbSbBS_4$. The radiation wavelength of the X-ray is λ = 1.5418 Å.