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New Chalcogenophosphates: $KBaPS_4$, $KBaPSe_4$, and $Ba_3PO_4PSe_4$

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Colourless single crystals of $KBaPS_4$ ($a = 11.587(2)$, $b = 6.700(1)$, $c = 10.118(2)$ Å), and pale orange ones of $KBaPSe_4$ ($a = 11.972(2)$, $b = 6.973(1)$, $c = 10.388(2)$ Å) were obtained by reactions of $Ba_3(PS_4)_2$ and $Ba_3(PSe_4)_2$, respectively, with KCl (790 °C; 30 h). The isotypic compounds crystallize with a slightly modified $TlEuPS_4$ type structure (*Pnma*, $Z = 4$); that is, the characteristic units are distorted discrete PX_4 tetrahedra (X: S, Se) interconnected by K^+ and Ba^{2+}. However, due to the strong distortion of the trigonal X_6 prisms along [001] the coordination numbers increase from 8 to 9 for the barium atoms and from 8 to 11 for the potassium atoms. Orange crystals of $Ba_3PO_4PSe_4$ ($a = 6.779(1)$, $b = 7.108(1)$, $c = 12.727(3)$ Å; $\alpha = 82.45(3)^\circ$, $\beta = 78.88(3)^\circ$, $\gamma = 81.34(3)^\circ$) resulted as a by-product of the synthesis of $Ba_3(PSe_4)_2$. The compound crystallizes in a new type of structure ($P\bar{1}$; $Z = 2$) and is the first chalcogenophosphate with discrete PO_4 and PSe_4 tetrahedra. The coordination polyhedra of the barium atoms are formed by both chalcogen atoms.

Key words: Chalcogenophosphates, Potassium, Barium, Crystal Structures