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Synthesis of novel lead–molybdenum and lead–tungsten oxyhalides with the pinalite structure, $Pb_3MoO_5Cl_2$ and $Pb_3WO_5Br_2$

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Abstract

Two new quaternary lead oxyhalides, $Pb_3MoO_5Cl_2$ and $Pb_3WO_5Br_2$, have been prepared. They are isostructural with the mineral pinalite, $Pb_3WO_5Cl_2$, and its barium analog. The crystal structure of $Pb_3MoO_5Cl_2$ has been refined from powder neutron diffraction data to $R_p = 0.0564$ and $R_{wp} = 0.0342$. All these structures contain significantly stretched MO_5 (M = Mo, W) square pyramids incorporated into the $[Pb_2O_2]$ sheets. Bond valence sums indicate significant overbonding of one of the metal sites, which increases along with structural distortions when passing from $Pb_3MoO_5Cl_2$ to $Pb_3WO_5Cl_2$ and from $Pb_3WO_5Cl_2$ to $Ba_3WO_5Cl_2$. Possibilities of preparing isostructural and structurally related compounds are discussed.

Keywords: $Pb_3MoO_5Cl_2$, pinalite, crystal structure, neutron diffraction