

Crystal structure of synthetic $\text{Al}_4\text{B}_2\text{O}_9$: A member of the mullite family closely related to boralsilite

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ABSTRACT

The crystal structure of $\text{Al}_4\text{B}_2\text{O}_9$, synthesized from $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{B}(\text{OH})_3$ via a sol-gel process, is studied and characterized by Rietveld refinements and grid search analyses combined with ^{11}B and ^{27}Al MAS NMR spectroscopy. The aluminum borate with a unit-cell composition of $\text{Al}_{12}\text{B}_6\text{O}_{72}$ is closely related to the boralsilite ($\text{Al}_{12}\text{B}_{12}\text{Si}_4\text{O}_{74}$) structure with Si replaced by B and to mullite ($\text{Al}_{4+2x}\text{Si}_{2-2x}\text{O}_{10-x}$). It crystallizes in the monoclinic space group $C2/m$, $a = 14.8056(7)$ Å, $b = 5.5413(2)$ Å, $c = 15.0531(6)$ Å, $\beta = 90.913(2)^\circ$, $Z = 8$ for $\text{Al}_4\text{B}_2\text{O}_9$. The main structural units are isolated chains of edge-sharing AlO_6 -octahedra running parallel to \mathbf{b} that is a characteristic feature of the mullite-type crystal structures. The octahedral chains are crosslinked by AlO_4 , AlO_5 , BO_3 , and BO_4 groups with two B atoms and one O atom ($\text{O}5'$) disordered on interstitial positions. ^{27}Al and ^{11}B NMR studies confirm the presence of sixfold (octahedral), fivefold, and fourfold (tetrahedral) coordinated Al (sixfold:[fourfold + fivefold] = ~50%:50%) and of threefold and fourfold coordinated B (~80%:20%).

Keywords: Aluminum borate, boron aluminate, $\text{Al}_4\text{B}_2\text{O}_9$, boralsilite, crystal structure, Rietveld refinement, MAS NMR spectroscopy