

Dimers $[\text{Al}_2\text{N}_6]^{12-}$ and Chains $\frac{1}{\infty} [\text{AlN}_{4/2}]^{3-}$ in the Crystal Structures of $\text{Ca}_6[\text{Al}_2\text{N}_6]$ and $\text{Ba}_3[\text{Al}_2\text{N}_4]$

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Dedicated to Prof. P. Böttcher on the occasion of his 60th birthday

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Nitridoaluminates, Preparation, Crystal Structure

Pale yellow transparent single crystals of $\text{Ca}_6[\text{Al}_2\text{N}_6]$ ($P2_1/c$, No. 14, $a = 693.7(3)$, $b = 614.9(3)$, $c = 987.1(5)$ pm, $\beta = 94.01(5)^\circ$; $Z = 4$) and colourless transparent single crystals of $\text{Ba}_3[\text{Al}_2\text{N}_4]$ ($Pnna$, No. 52, $a = 617.9(2)$, $b = 1005.2(4)$, $c = 1023.0(4)$ pm; $Z = 4$) were obtained from reactions of mixtures of the representative metals with nitrogen at $T_{\text{max}} = 1000^\circ\text{C}$. The crystal structure of $\text{Ca}_6[\text{Al}_2\text{N}_6]$ contains isolated units $[\text{Al}_2\text{N}_6]^{12-}$ built of two edge-sharing tetrahedra. $\text{Ba}_3[\text{Al}_2\text{N}_4]$ is an isotype of $\text{Sr}_3[\text{Al}_2\text{N}_4]$. The crystal structure contains infinite chains $\frac{1}{\infty} [\text{AlN}_{4/2}]^{3-}$ of trans edge-sharing tetrahedra.

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