The Last Missing Member of the $AE_2[BN_2]Cl$ Series – Synthesis, Structural and Spectroscopic Characterization of $Ba_2[BN_2]Cl$

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Pale grey-blue, transparent single crystals of $Ba_2[BN_2]Cl$ ($I4_132$ (no. 214), $a = 1462.88(1)$ pm, $Z = 24$) are obtained by the reaction of $Ba$, $BaCl_2$, $BN$ and $NaN_3$ in arc-welded Ta ampoules at $1200$ K. The crystal structure was determined by single crystal X-ray structure analysis. The Raman and IR spectra of the title compound show the expected fundamental frequencies ($\nu_s = 1038$; $\nu_{as} = 1969$ and 2087; $\delta = 616 / 636$ cm$^{-1}$) for a nitridoborate unit with $D_{oh}$ symmetry. The [N–B–N] structure obtained by X-ray single crystal structure determination corroborates this finding within the standard deviations of the measurement with $d(B–N) = 132.3(8)$ pm and $\angle(N–B–N) = 178.5(13)^\circ$. Our results compare well to the data reported for cubic and orthorhombic $Ba_3[BN_2]_2$ as well as to the isotypic compound $Ba_2[BN_2]Br$.

Key words: Barium, Chloride, Nitridoborate, Nitride, Structure Elucidation, IR Spectroscopy, Raman Spectroscopy