

Ba₉[NbN₄]₂O[CN₂] – Synthesis, Crystal Structure and Raman Spectrum

Olaf Reckeweg and Francis J. DiSalvo

Baker Laboratory, Department of Chemistry and Chemical Biology, Cornell University,
Ithaca, NY 14853-1301, USA

Reprint requests to Dr. O. Reckeweg. E-mail: olaf.reykjavik@gmx.de

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Red transparent single crystals of Ba₉[NbN₄]₂O[CN₂] were synthesised by the reaction of BaO coated Ba metal, C and Nb powder in arc-welded Nb ampoules at 1300 K. The title compound was characterised by X-ray single crystal diffraction ($P\bar{1}$, $a = 799.05(2)$, $b = 962.61(2)$ and $c = 1264.38(4)$ pm; $\alpha = 75.859(1)$, $\beta = 85.745(1)$ and $\gamma = 87.8621(8)^\circ$; $Z = 2$) and Raman spectroscopy ($\nu_{\text{sym}} = 1234$ and $\delta = 632/658/668 \text{ cm}^{-1}$). It now seems likely that a nitride-azide compound we previously reported, Ba₉[NbN₄]₂N[N₃], does not exist, but is in fact the title compound.

Key words: Cyanamide, Nitride, Structure Elucidation