

Synthesis, Crystal Structure and Optical Spectra of $\text{Yb}_2[\text{CN}_2]_3$

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Red-orange, transparent single crystals of $\text{Yb}_2[\text{CN}_2]_3$ [trigonal, $R\bar{3}c$ (no. 167), $a = 630.02(3)$ and $c = 2947.4(2)$ pm, $Z = 6$] are obtained by the reaction of Yb, Sn, $\text{Zn}[\text{CN}_2]$ and NaN_3 in arc-welded Nb ampoules at 1100 K. The title compound exhibits characteristic C–N bond lengths and angles [$d(\text{C–N}) = 122.7(3)$ pm and $\angle(\text{N–C–N}) = 178.4(5)^\circ$, respectively] within the $[\text{N}=\text{C}=\text{N}]^{2-}$ unit as well as the expected fundamental frequencies in its optical spectra (Raman: $\nu_s = 1338$; $\delta = 643 / 683 / 695 \text{ cm}^{-1}$; IR: $\nu_{as} = 2005 / 2037$; $\delta = 640 / 679 \text{ cm}^{-1}$). Since $\text{Yb}_2[\text{CN}_2]_3$ adopts a corundum-type structure, Yb^{3+} is octahedrally coordinated by six N atoms of different $[\text{CN}_2]^{2-}$ anions [$d(\text{Yb–N}) = 228.6(3)$ and $233.4(3)$ pm, $3 \times$ each] and every $[\text{CN}_2]^{2-}$ group has four Yb^{3+} as next neighbours which form a distorted tetrahedron.

Key words: Trivalent Ytterbium, Carbodiimide, Cyanamide, Crystal Structure, Optical Spectroscopy