

A Novel Method for Synthesizing Crystalline Copper Carbodiimide, CuNCN. Structure Determination by X-Ray Rietveld Refinement

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Well-crystallized copper carbodiimide, CuNCN, was synthesized by the slow oxidation of a copper(I) cyanamide precursor under aqueous conditions. The X-ray powder data evidence the orthorhombic system and space group *Cmcm* with $a = 2.9921(1)$, $b = 6.1782(1)$, $c = 9.4003(2)$ Å, $V = 173.769(5)$ Å³ and $Z = 4$. There is a strongly distorted octahedral Cu²⁺ coordination reflecting a typical first-order Jahn-Teller effect, with interatomic distances of $4 \times \text{Cu-N} = 2.001(2)$ Å and $2 \times \text{Cu-N} = 2.613(3)$ Å; the NCN²⁻ unit adopts the carbodiimide shape with C-N = 1.227(4) Å. Despite the formal d^9 electron count of Cu²⁺, CuNCN exhibits a small temperature-independent paramagnetism and is likely to be a metallic conductor.

Key words: Copper, Cyanamide, Carbodiimide, Rietveld Refinement, Jahn-Teller Distortion