Synthesis, Thermal and X-Ray Investigations of the High-Temperature Phase of Copper(I) Cyanide

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CuCN was investigated by chemical analysis, IR spectroscopy and powder X-ray diffraction. A high-temperature phase of CuCN was identified and structurally characterized by Rietveld refinement. HT-CuCN is isotypic to AgCN (*R*3*m* (No. 166), $Z = 3$, $a = 597.109(8)$, $c = 484.33(5)$ pm, Cu (3a), C/N (6c), $z = 0.3915(10)$ at 77 K) with head-tail disorder of the cyanide anions.

Key words: Copper, Cyanide, Structure Elucidation, Thermal Properties, Optical Spectroscopy