

Catalytic Formation and Crystal Structure of Cyanoguanylurea

$\text{H}_2\text{NC}(=\text{O})\text{NHC}(\text{NH}_2)\text{NCN}$

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Z. Naturforsch. **60b**, 377 – 382 (2005); received December 15, 2004

The ion exchange reaction between ammonium cyanoureate $\text{NH}_4[\text{H}_2\text{NC}(=\text{O})\text{NCN}]$ and zinc chloride yielded single crystals of the urea derivative cyanoguanylurea $\text{H}_2\text{NC}(=\text{O})\text{NHC}(\text{NH}_2)\text{NCN}$, which was obtained as a by-product alongside zinc cyanoureate and traces of ammonium chloride. It is assumed that owing to its Lewis and Brønsted acidity, the hydrated Zn^{2+} ion acts as a catalyst, promoting the degradation of the cyanoureate anion with subsequent formation of the title compound. The crystal structure was solved in the centrosymmetric space group $P2_1/n$ ($a = 476.7(1)$, $b = 965.3(2)$, $c = 1165.6(2)$ pm, $\beta = 97.75(3)^\circ$, $V = 531.4(2) \cdot 10^6 \text{ pm}^3$, $Z = 4$, $T = 200 \text{ K}$). In the solid there are non-planar cyanoguanylurea molecules with a dicyandiamide-type C-N system, building up a layered structure with sparse interlayer contacts and significant hydrogen bonding within the layers.

Key words: Zinc Catalysis, Crystal Structure, Cyanourea