Crystal structure and thermochemical reactivity of an unusual copper complex that contains copper in four different coordination geometries

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Dedicated to Prof. Volker Staemmler on the occasion of his 65\(^{th}\) birthday

According to X-ray single crystal structure analysis, \(\left\{\text{Cu}^{II}(en)_2\right\}_2\left[\text{Cu}^{I}(\text{CN})_6\right]\left[\text{Cu}^{II}(en)_2\right]\left[\text{Cu}^{I}(\text{CN})_3\right] \cdot 2\text{H}_2\text{O}\) contains copper in four different coordination environments: trigonal-planar, square-planar, square-pyramidal, and tetrahedral. The different coordination geometries of copper were investigated by quantum chemical calculations of model compounds, thus allowing to tentatively assign the different CN-bands in the infrared spectrum. The thermolysis led to sub-µm-sized rod-like copper(II)oxide particles.