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

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According to X-ray single-crystal structure analysis, $\{[Cu^{II}(en)_2]_2[Cu^{I}_2(CN)_6]\}[Cu^{II}(en)_2]_2[Cu^{I}(CN)_3]_2 \cdot 2H_2O$ 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 IR spectrum. The thermolysis led to sub-μm sized rod-like copper(II) oxide particles.