

SUPPORTING INFORMATION

Title: Copper(I) and Iron(II) Complexes of a Novel Tris(pyridyl)ethane-Derived N₄ Ligand: Aspects of Redox Behaviour and Bioinorganic Physicochemistry

Author(s): D. Wiedemann, E. Świętek, W. Macyk, A. Grohmann*

Ref. No.: Z201300112

Copper(I) and Iron(II) Complexes of a Novel Tris(pyridyl)ethane-Derived N4 Ligand: Aspects of Redox Behaviour and Bioinorganic Physicochemistry

Dennis Wiedemann, Elżbieta Świątek, Wojciech Macyk, and Andreas Grohmann*

Supporting Information

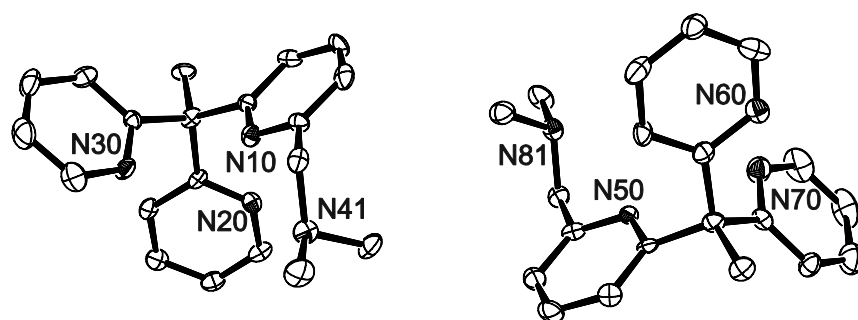


Figure S1. Crystal structure of 1-{6-[1,1-di(pyridin-2-yl)ethyl]pyridin-2-yl}-*N,N*-dimethylmethanamine trihydrobromide—water(4/3) ($1 \cdot 3 \text{ HBr} \cdot \frac{3}{4} \text{ H}_2\text{O}$). ORTEP representation with 50 % probability ellipsoids, hydrogen atoms, bromide ions and water molecules omitted for clarity. All nitrogen atoms except for N10 and N50 are protonated. In order to give physically meaningful ADPs, *ipso*-carbon atoms in rings had to be treated with very tight ISOR restraints.

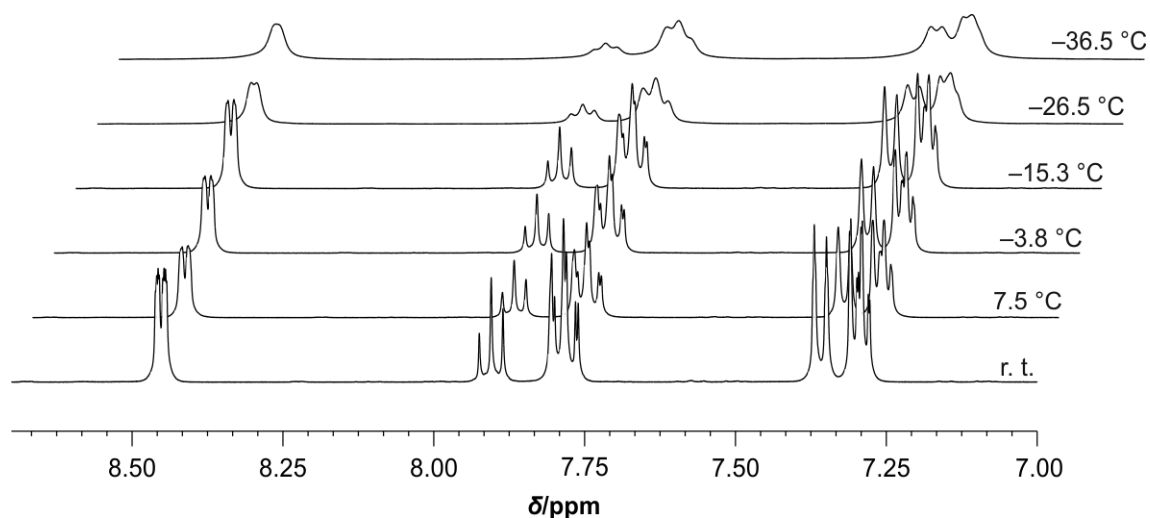


Figure S2. Variable-temperature ^1H -NMR spectra of $[\text{Cu}^{\text{I}}\text{L}(\text{MeCN})]\text{PF}_6$ (**2**) in CD_3CN at 400 MHz (range of aromatic protons).