Crystal Structure, Spectroscopic and Redox Properties of Copper(II) Bis{2-[(2,6-dimethylphenyl)iminomethyl-3-methoxyphenolate]}

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The coordination chemistry of N-(2,6-di-methylphenyl)-2-hydroxy-3-methoxybenzaldimine (1) with Cu(II) has been investigated by X-ray crystallography, electronic and EPR spectroscopies, as well as by electro- and magnetochemistry. The title complex 2 crystallizes in the orthorhombic space group $P2_12_12_1$ (a=8.1538, b=17.7466, c=19.8507 Å). The mononuclear square-planar molecules 2 featuring trans-N₂O₂ coordination are connected via weak intermolecular C-H··· π interactions into infinite chains parallel to the a axis. Although the intermolecular Cu···Cu separations within individual chains and between chains are very long (8.154 and 9.726 Å), the exchange interaction parameter G=2.03 < 4, estimated from solid state EPR spectra, suggests the existence of long-distance superexchange pathways between adjacent Cu(II) centers. The electronic and electrochemical features of the compound are also discussed.

Key words: Crystal Structure, $C-H\cdots\pi(Ph)$ Bonding, Superexchange