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Synthesis, characterisation and electrochemistry of eight Fe coordination compounds containing substituted 2-(1-(4-R-phenyl-1H-1,2,3-triazol-4-yl)pyridine ligands, R = CH₃, OCH₃, COOH, F, Cl, CN, H and CF₃

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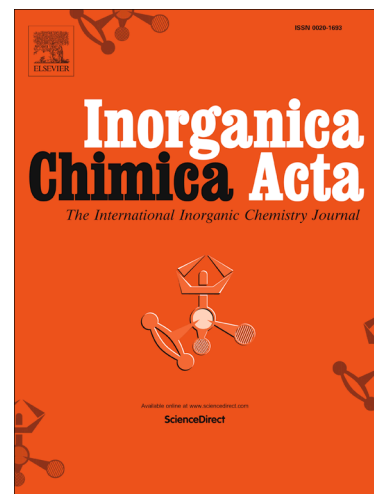
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Synthesis, characterisation and electrochemistry of eight Fe coordination compounds containing substituted 2-(1-(4-R-phenyl)-1H-1,2,3-triazol-4-yl)pyridine ligands, R = CH₃, OCH₃, COOH, F, Cl, CN, H and CF₃.

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Abstract

Eight different Dichloro(bis{2-[1-(4-R-phenyl)-1H-1,2,3-triazol-4-yl]-N³}pyridine-N)}iron(II) compounds, **2** – **9**, have been synthesised and characterised, where group R = CH₃ (L²), OCH₃ (L³), COOH (L⁴), F (L⁵), Cl (L⁶), CN (L⁷), H (L⁸) and CF₃ (L⁹). The single crystal X-ray structure was determined for the L³ which was complemented with Density Functional Theory calculations for all complexes. The structure exhibits a distorted octahedral geometry, with the two triazole ligands coordinated to the iron centre positioned in the equatorial plane and the two chloro atoms in the axial positions. The values of the Fe^{II/III} redox couple, observed at *ca.* –0.3 V versus Fc/Fc⁺ for

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