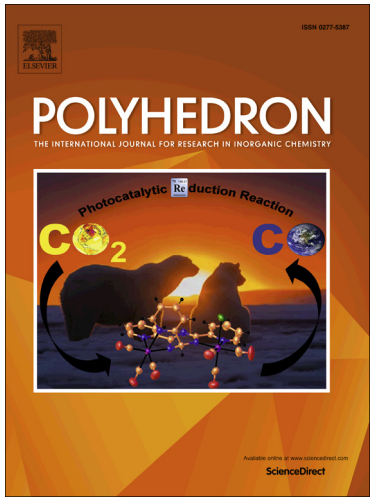

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Evaluation of Iron(III)-N(amine)$_2$N(py)$_2$ Complexes as Potential Bioreductively Activated Carriers for Naphthoquinone-based Drugs

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Abstract

Two new iron(III) complexes, [Fe(bhnq)(L1)]$NO_3 \cdot CH_3OH \cdot 2H_2O$ (**1**) and [Fe(bhnq)(L2)]$ClO_4.CH_3OH$ (**2**) (L1 = *N,N'*-bis(pyridin-2-ylmethyl)ethylenediamine and L2 = *N,N'*-dimethyl-*N,N'*-bis(pyridin-2-ylmethyl)ethylenediamine), were investigated as potential candidates for bioreductively activated prodrugs. These complexes present a distorted octahedral structure with 2,2'-bis(3-hydroxy-1,4-naphthoquinone), $(bhnq)^{2-}$, coordinated in a bidentate fashion to the iron(III) ion. A reversible wave associated with the Fe^{3+}/Fe^{2+} couple was observed in MeCN for **1** and **2** respectively at -0.05 V and 0.01 V *vs* SHE. Unlike previously studied cobalt(III)-based analogs and one iron(III) platform that showed efficient bioreductive activation, complexes **1** and **2** undergo fast dissociation in aqueous buffered solutions with immediate release of the $bhnq^{2-}$ ligand. Therefore, we conclude that the labile $3d^5$ iron(III) ion is a limited bioreducible carrier for naphthoquinone-based prodrugs when coordinated to this [$N_2N^{Py}_2$] platform. Considerable modification of the current ligands or the meticulous selection of other alternative ligand platforms may be necessary to attain this goal.