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Correction to Characterization of the Fleeting Hydroxoiron(III) Complex of the Pentadentate TMC-py Ligand

Wei-Min Ching, Ang Zhou, Johannes E. M. N. Klein, Ruixi Fan, Gerald Knizia, Christopher J. Cramer,* Yisong Guo,* and Lawrence Que, Jr.*

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Page 11129. The first two sentences of the paragraph in the right column state that "Masuda and Borovik have reported the only crystal structures of nonheme hydroxoiron(III) complexes.[11−13] These complexes have been stabilized by the introduction of H-bonding moieties in the second coordination sphere in the design of the supporting ligand (Figure 1)." These sentences should be replaced by the following text in order to reflect the larger number of crystal structures of $Fe^{III}(OH)$ complexes that have been reported. We apologize for this unfortunate oversight.

"There are a number of mononuclear nonheme hydroxoiron(III) complexes for which crystal structures have been solved. The first crystal structures of such species (Figure 1) were reported by Masuda[1,2] and Borovik,[3−5] having Fe−OH bond lengths of 1.876(2) Å for $[Fe^{III}(OH)(L1)(RCO_2)](ClO_4)$ [L1 = tris(6-neopentylamino-2-pyridylmethyl)amine] and 1.9264(17) Å for $K[Fe^{III}(OH)(H_3L2)]$ [H_6L2 = tris(*N*′-*tert*-butylureaylato-*N*-ethylamine)], respectively. Subsequent additions to this list include K[Fe(OH)(L3)] [d_{Fe-OH} = 1.877(3) Å; H_3L3 = tris(*N*-isopropylcarbamoylmethylamine)], $K[Fe^{III}(OH)(L4)]$ [d_{Fe-OH} = 1.886(1) Å; H_3L4 = (*N*′-*tert*-butylureaylato-*N*-ethylbis(*N*″-isopropylcarbamoylmethyl)amine], and $Me_4N[Fe^{III}(OH)(L5)]$ [d_{Fe-OH} = 1.831(1) Å; H_3L5 = *N*,*N*′,*N*″-[2,2′,2″-nitrilotris(ethane-2,1-diyl)]tris(4-methylbenzenesulfonamide)], which were determined by Borovik,[6,7] $Q[Fe^{III}(OH)(L6)]$ [d_{Fe-OH} = 1.856(11) and 1.863(5) Å for Q = $[K(DMF)_3]^+$ and H_3O^+, respectively; H_3L6 = $[(4\text{-}t\text{-}BuC_6H_4)NH(o\text{-}C_6H_4)]_3N$], which were obtained by Stavropoulos,[8] $K[Fe^{III}(OH)(L7)]$ [d_{Fe-OH} = 1.867(2) Å; H_3L7 = tris(5-mesityl-2-pyrrolylmethyl)amine] and $[Fe^{III}(OH)(L8\text{ or }L9)](OTf)_2$ [d_{Fe-OH} = 1.837(3) and 1.835(2) Å, respectively; L = *N*,*N*-bis(2-R-6-pyridylmethyl)-*N*-bis(2-pyridyl)methylamine, where R = neopentyl-NH for L8 and R = phenyl-NH for L9], which were reported by Chang.[9,10] In most of the structures, H-bond donors introduced into the second coordination spheres of the supporting ligands interact with the $Fe^{III}(OH)$ unit, while the $Fe^{III}(OH)$ unit serves as a H-bond donor to a bound carboxylate in the L1 complex and to a sulfonamide functionality on the supporting polydentate ligand in the L5 complex. No H-bonding interactions were observed for the L3 and L7 complexes. These structures show that the Fe^{III}−O bond distance can range from 1.83 to 1.93 Å."

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