

New complexes Fe(III) with mixed anion ligands

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The chemistry of iron complexes is investigated recently since these is present in various biological redox systems including peroxidases, catalyses, superoxide dismutases, dioxygenases and lipoxidases. Pyridinecarboxylic acids are present in many natural products, such as alkaloids, vitamins and enzymes, so their metal complexes can be used as models in many research fields. The dicarboxylic acid analogue especially pyridine-2,6-dicarboxylic acid (dipicolinate acid) is one of the most suitable ligand systems for modeling potential metallo-pharmaceutical compounds because of its low toxicity, amphiphilic nature and diverse biological activities. Anion NCS⁻ as ligand may be bonded in complexes of eleven possible manners. In Cambridge Crystallographic Data Base are 997 crystal structure where NCS groups are bonded through nitrogen atom. But in Cambridge Crystallographic Data Base there is neither one structure that would include these two anionic ligands.

This contribution present black complexes of compositions (cat)₂[Fe^{III}(η^3 -dipic)(NCS)₃] (cat = (H-qui)(**1**); (H-3-meiq)(**2**); (H₂-4,4-bipy)(**3**), (H-3-meiq)₄[Fe^{III}(η^3 -dipic)(NCS)₃]₂(**4**) and (H-2-pic)₂[Fe^{III}(η^3 -dipic)(H₂O)(NCS)₂](**5**) (H-qui = quinolinium; H-3-meiq = 3-methylisoquinolinium; H₂-4,4-bipy = 4,4-bipyridinium; H-2-pic = 2-picolinium) were prepared and studied by X-ray analyses. Each Fe(III) atom has pseudo-octahedral arrangement created by terdentate dipic - ¹O, ²N, ³O ligand and three monodentate NCS ligands in complexes (**1** - **4**) and one H₂O plus two NCS ligands in (**5**). Each dipic - ¹O, ²N, ³O forms a pair of five-membered metallocyclic rings (¹OC₂²NC₂³O) with the mean value of O - Fe - N bite angles of 75,5°. The inner coordination sphere FeO₂N₄ (**1** - **4**) and FeO₃N₃ (**5**) are unsymmetric, because one side is build up by terdentate dipic ligand and other one by three monodentate (NCS)₃ (**1** - **4**) or H₂O+(NCS)₂ (**5**) donor ligands.

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