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Preparation, Spectroscopic and Structural characterization of the hexa-coordinate, high-spin iron(III) carbonato « picket fence » porphyrin complex Mondher Dhifet, Mohamed Salah Belkhiria et Habib Nasri, *Laboratoire de Physico-Chimie des Matériaux, Faculté des Sciences de Monastir, Avenue de l'environnement, 5019 Monastir, Tunisie.*
E-mail: mondherdhifet_2005@yahoo.fr

Keywords: metalloporphyrins, carbonato-complexes, Heme model.

The preparation and characterization of the (carbonato)($\alpha,\alpha,\alpha,\alpha$ -tetrakis(*o*-pivalamidophenyl)porphyrinato)iron(III) complex is described. The synthesis procedure utilizes the cryptand-222 to solubilize potassium carbonate. The compound has been characterized by UV-vis, IR and ^1H NMR spectroscopies. Proton NMR data for the isolated product is in accordance with high-spin ($S = 5/2$) ferric porphyrin species. The X-ray molecular structure of this species has been also determined. The iron atom is hexa-coordinated by the four nitrogen atoms of the pyrrol rings and the two oxygen atoms of the CO_3^{2-} group. It lies at 0.695(1) Å out of the porphyrinato plane and 0.640(1) Å out of the four nitrogen plane. The Fe-O bond length is 2.067(10) Å and the average Fe-Np distance is 2.076(10) Å with is a stereochemical proof that the $[\text{Fe}^{\text{III}}(\text{TpvPP})(\text{CO}_3)]^+$ is high-spin. Crystal data for $[\text{K}(222)][\text{Fe}(\text{TpvPP})(\text{CO}_3)]\cdot\text{C}_6\text{H}_5\text{Cl}\cdot 2\text{H}_2\text{O}$ are: $a = 18.085(5)$ Å ; $b = 21.505(10)$ Å ; $c = 23.160(5)$ Å ; $\beta = 100.52(3)^\circ$, monoclinic, space group $\text{P2}_1/\text{n}$; $V = 8855$ Å³ ; $Z = 4$; 27435 unique reflections measured which were used in all refinements. The final agreement factors $R(F)$ ($I > 2\sigma(I)$) for 18421 reflections and $wR(F^2)$ (all data) were 0.09 and 0.21, respectively.

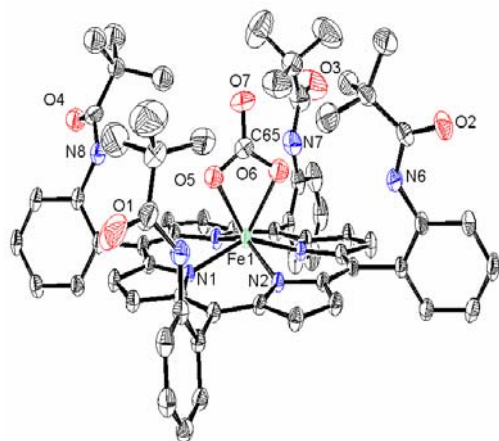


Fig. *ORTEP* diagram of $[\text{Fe}(\text{TpvPP})(\text{CO}_3)]^+$ ion complex showing thermal ellipsoids at 30 % probability level.

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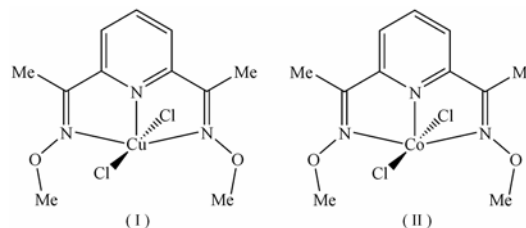
Copper(II) and cobalt(II) complexes of 2,6-diacetylpyridine bis(*O*-methyloxime) Muharrem Dinçer^a, Namık Özdemir^a, Osman Dayan^b, Bekir Çetinkaya^b, ^a*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139, Samsun, Turkey.* ^b*Department of Chemistry, Faculty of Science,*

Ege University, 35100, İzmir, Turkey.

E-mail: mdincer@omu.edu.tr

Keywords: crystal structure analysis, coordination complexes, catalysts

The title complexes, dichloro[(1*E*,1'*E*)-1,1'-(pyridine-2,6-diyl)diethanone bis(*O*-methyloxime)- $\kappa^3\text{N}^1,\text{N}^2,\text{N}^6$]copper(II), $[\text{CuCl}_2(\text{C}_{11}\text{H}_{15}\text{N}_3\text{O}_2)]$, (I), and dichloro[(1*E*,1'*E*)-1,1'-(pyridine-2,6-diyl)diethanone bis(*O*-methyloxime)- $\kappa^3\text{N}^1,\text{N}^2,\text{N}^6$]cobalt(II), $[\text{CoCl}_2(\text{C}_{11}\text{H}_{15}\text{N}_3\text{O}_2)]$, (II), crystallize in space groups $\text{P2}_1/\text{c}$ [1] and Pnma [2], respectively. In each compound, the metal atom is pentacoordinated by the two methyloxime N atoms, one pyridine N atom and two Cl atoms. Although the coordination polyhedra around the metal atom in (I) is a strongly distorted trigonal-bipyramid, the coordination polyhedra in (II) is a strongly distorted square-bipyramid. It is observed that the N(oxime)-M-N(pyridine) bond angle for five-membered chelate rings of 2,6-diacetylpyridine dioxime complexes is inversely related to the magnitude of the M-N(pyridine) bond. Both structures are stabilized by intra- and intermolecular C-H...Cl hydrogen bonds. Despite the similar chemical compositions of the Cu^{II} and Co^{II} complexes, the packing patterns of the molecules in the crystal structures are quite different. In contrast to the columnar packed structure observed in (I), the molecules of (II) pack in layers.



[1] Özdemir N., Dinçer M., Dayan O. & Çetinkaya B., *Acta Cryst.*, 2006, C62, m315-m318.

[2] Özdemir N., Dinçer M., Dayan O. & Çetinkaya B., *Acta Cryst.*, 2006, C62, m398-m400.

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Structural Study of Dendronized Palladium Scorpionate Complexes. Pilar Gómez-Sal, Alberto Sánchez-Méndez, Ernesto de Jesús, Juan C. Flores, *Departamento de Química Inorgánica, Universidad de Alcalá, Alcalá de Henares (Madrid) Spain.*
E-mail: pilar.gomez@uah.es

Keywords: crystal and molecular structure; dendrimers; palladium compounds.

Most dendrimers are flexible molecules and therefore their structures have been largely debated. Several computational and experimental techniques have been used to gain structural information regarding dendrimers in solution and the solid state, but only X-ray diffraction techniques allow the acquisition of highly precise data regarding the internal molecular conformations. Unfortunately, the growth of single crystals of suitable quality has been restricted mainly to small dendrimers because of a variety of problems, in part due to the conformational flexibility of these molecules [1]. Poly