

= 16.780(3) Å,  $c = 10.0559(16)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 90.504(3)^\circ$ ,  $\gamma = 90^\circ$ , and  $Z = 2$ . These parameters suggested a monoclinic unit cell. This Ligand has a monoclinic crystal system and it can be seen there are  $\pi$ - $\pi$  stacking interaction between both naphthalene and pyridin groups. The N...N separation between the pyridyl groups in L is 15.3 Å.

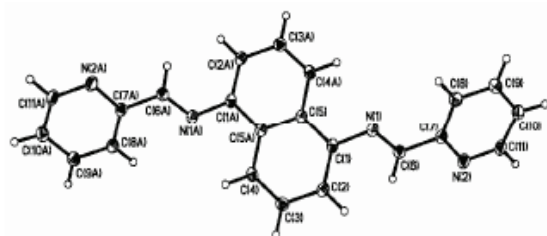


Fig 1. ORTEP of (2-py)-CH=N-C10H6-N=CH-(2-py)

[1] G.F.Swieger, T.J. Malefetse, *Chem. Rev.* 100, 2000, 3483. [2] M. J. Zaworotko, *Chem. Soc. Rev.* 1994, 283.

**Keywords:** schiff-base; monoclinic; naphthalene

#### FA4-MS06-P22

**Crystal Structures of  $\mu$ -bridged Trinuclear and Polynuclear Cadmium Metal Complexes.** Orhan Atakol<sup>a</sup>, Dinçer Ülkü<sup>b</sup>. <sup>a</sup>Ankara University Chemistry Department, Ankara-Turkey, <sup>b</sup>Hacettepe University Physics Department, Ankara-Turkey.

E-mail: [atakol@science.ankara.edu.tr](mailto:atakol@science.ankara.edu.tr)

Linear and angular homo- or heteronuclear metal complexes based on Schiff base ligands are of interest because of their magnetic super-exchange interactions between bridged metal ions [1]. In these complexes, various combinations of metal ions in the central and terminal locations, as well as the  $\mu$ -bridges, such as acetate or nitrite anions, are possible. The two new tri- and polynuclear structures described here are an extension of our previous structural studies [2] of bridged metal complexes.

(I)  $[\text{C}_{44}\text{H}_{54}\text{CdCu}_2\text{N}_{12}\text{O}_4]$ , Pccn,  $a = 13.8382(12)$ ,  $b = 15.3944(11)$ ,  $c = 22.5753(13)$  Å,  $Z = 4$ ,  $D_x = 1.46$  g.cm<sup>-3</sup>,  $\lambda = 0.71073$  Å,  $I > 2\sigma$  4229,  $N_{\text{par}} = 295$ ,  $R_w \rightarrow 0.028, 0.061$ ,  $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}} \rightarrow 0.27, -0.27$  e Å<sup>-3</sup>. The central metal atom Cd has an octahedral environment consisting of four bridging O atoms from the ligand and two N atoms from the azide groups. The terminal Cu atoms have square-pyramidal coordination, involving two N and two O atoms from a ligand and one O atom from a dimethyl formamide group. The bridging angle Cd-O-Cu between the central and terminal metal atoms is 74.87(2)°. The Cd...Cu and Cu...Cu distances are 3.3239(5) and 4.0412(6) Å, respectively.

(II)  $[\text{C}_{38}\text{H}_{40}\text{Cd}_2\text{I}_4\text{N}_4\text{O}_4]$ , P1̄,  $a = 10.3890(12)$ ,  $b = 13.1950(11)$ ,  $c = 16.2350(13)$  Å,  $Z = 2$ ,  $D_x = 2.07$  g.cm<sup>-3</sup>,  $\lambda = 0.71073$  Å,  $I > 2\sigma$  8239,  $N_{\text{par}} = 465$ ,  $R, R_w \rightarrow 0.08, 0.175$ ,  $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}} \rightarrow 1.30, -1.88$  e Å<sup>-3</sup>. Cd atom has a distorted tetrahedral coordination consisting of two O atoms from two neighbouring ligands and two I atoms. The O atoms in the Cd coordination sphere belonging to two different ligands lead to polymerisation. It is actually a molecular  $\mu$  bridge connecting the Cd atoms

via phenolic oxygens. The Cd-I bond distances range from 2.6980(14) to 2.7547(14) Å.

[1] Fukuhara C., Tsuneyoshi K., Matsumoto N., Kida S., Mikuriya M., Mori M. *J. Chem. Soc. Dalton Trans.* 1990, 3473. [2] Arıcı C., Ercan F., Atakol O., Akay A., Ülkü D., *Acta Cryst.* 1999. C55, 928-930

**Keywords:** metalloorganic structures; coordination compounds; polynuclear complexes

#### FA4-MS06-P23

**Synthesis and Spectroscopic Properties of a Five Coordinate Cyanato Iron(II) “Picket Fence” Porphyrin Complex.** Mondher Dhifet<sup>a</sup>, Mohamed Salah Belkhiria<sup>a</sup>, Jean-Claude Daran<sup>b</sup>, Habib Nasri<sup>a</sup>. <sup>a</sup>Laboratoire de Physico-Chimie des Matériaux, Faculté des Sciences de Monastir, Avenue de l'Environnement, 5019 Monastir, Tunisia. <sup>b</sup>Laboratoire de Chimie de Coordination, UPR CNRS 8042, 205 route de Narbonne, 31077 Toulouse cedex, France.

E-mail: [mondherdhifet\\_2005@yahoo.fr](mailto:mondherdhifet_2005@yahoo.fr)

The reaction of four-coordinate picket fence iron(II) porphyrin complex [Fe(TpivPP)] with cryptand-222 solubilized NaOCN in organic solvents, yields the five-coordinate porphyrin species [Fe(TpivPP)(NCO)]<sup>-</sup>. The five-coordinate, high-spin ( $S = 2$ ) (cyanato-*N*)( $\alpha, \alpha, \alpha, \alpha$ -tertakis(*o*-pivalamidophenyl) porphinato)iron(II) “picket fence” porphyrin derivative [Na(222)][Fe(TpivPP)(NCO)] has been synthesized and characterized by UV-vis, IR and magnetic susceptibility spectroscopies as well as single-crystal structure determinations. The X-ray molecular structure of the chlorobenzene solvate of the metalloporphyrin derivative has been determined. The  $S = 2$  spin state has also been confirmed from the measurement of the temperature-dependant magnetic susceptibility. [Na(222)][Fe(TpivPP)(NCO)] crystallize in the monoclinic system with  $a = 24.0027(8)$  Å;  $b = 14.7581(6)$  Å;  $c = 23.6448(8)$  Å;  $\beta = 106.078(2)^\circ$ ;  $V = 8048.18(49)$  Å<sup>3</sup>,  $T = 180$  K, space group C2,  $Z = 4$ ,  $\mu$  (Mo-K $\alpha$ ) = 0.258 mm<sup>-1</sup>. 18133 unique reflections measured ( $R_{\text{sigma}} = 0.0496$ ) which were used in all refinements. The final agreement factors  $R(F)$  ( $I > 2\sigma(I)$ ) for 14508 reflections and  $wR(F^2)$  (all data) were 0.0602 and 0.1631, respectively. The average Fe-Np bond distance is 2.121(1) Å. The iron atom is pentacoordinated by the four nitrogen atoms of the pyrrole rings and the nitrogen atom of the NCO<sup>-</sup> group. It lies at 0.7096(9) Å out of the porphinato plane and 0.5940(15) Å out of the four nitrogen plane of the porphyrin ring. The Fe-N(NCO) bond length is 2.007(2) Å and the Fe-N-C(NCO) bond angle is 176.62(7)°.

The Figure 1 is an ORTEP diagram of the [Fe(TpivPP)(NCO)]<sup>-</sup> complex.