MS27 P04

Synthesis and structures of Nickel complexes derivative from Dehydroacetic acid Amel Djedouani[a], Abderrahmen Bendaas[a], Magali Allain[b], Gilles Bouet[c] and Mustayeen Khan[c] [a]*Laboratoire d'Électrochimie des Matériaux Moléculaires et Complexes, Université Farhat Abbés de Sétif,* [b]*CIMM, CNRS UMR 6200, Faculté des Science, Angers Cedex, France,,* [c]*SONAS, EA 921, Université D'Angers, Faculté de Pharmacie, Angers Cedex, France*. E-mail: Djed_amelle@yahoo.fr

Keywords : Dehydroacetic acid, Complexes, Nickel

Mixed d-transition metal diketone compounds were used extensively as starting materials in the early days of metallocene chemistry [1]. Dehydroacetic acid or [DHA : 3-Acetyl-6-methyl-2H-Pyran-2,4(3H)-dione], Is an industrially product used as a fungicide, a bactericide and also as an important intermediate in organic synthesis, usually obtained through the auto-condensation of ethyl acetoacetate [2], However, little is known on ils metal complexes. The Cu and Zn complexes have been reported to be, respectively, a fungicide and a heat stabilizer for vinyl chloride resins [3]. This has motivated our study of the structural characterization of nickel complexes of dehydroacetic acid. We present here the Synthesis, and crystal structures determination of the mononuclears complexes, Bis[3-acetyl-6-methyl-2H-pyran-2,4(3H)-dionato]bis(dimethyl formamide)nickel(II); $[Ni(DHA)_2.2DMF]$ (1) and Bis[3-acetyl-6-methyl-2H-pyran-2,4(3H)-dionato]bis(dimethyl sulfoxide)nickel(II); $[Ni(DHA)_2.2DMSO]$ (2), with (DMF is dimethylformamide and DMSO is dimethylsulfoxide). Cristals, were mounted on a CCD area detector equipped with graphite-monochromated Mo Kα (λ = 0.71073 Å) radiation at 293 K, using the ω/2θ scan mode. (1) has the following structural properties : triclinic, P-1, a = 7.764(2), b = 8.227(2), c = 9.549(2) Å, α = 85.03(2)°, β = 85.99(2)°, γ = 78.23(2)°, V = 594.0(2) $Å^3$. and Z = 2. Complex (2), crystallize in the monoclinique space group $P2_1/n$ with a = 11.385(10), b = 6.2833(4), c = 16.4660(10) Å, β = 91.673(7)°, V = 1177.40(15) $Å^3$ and Z = 4. The metal atoms are, located on an inversion centre, and have an octahedral coordination geometry of type MO_6, surrounded by two bidentates dehydroacetic acid. DHA ligands occupy the equatorial plane of the complex in a trans configuration. The two axial positions are occupied by oxygen atoms of molecules of solvant (DMF or DMSO). The packing of the complexes are stabilized by weak intermolecular C—H…O hydrogen bonds, which form a a two-dimensional and a three-dimensional network, for (1) and (2) respertively.

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MS27 P05

Molecular Structure of (E)-3-[(2bromophenylimino)methyl] benzene-1,2-diol, (I) and (E)-3-[(2-(trifluoromethyl) phenylimino)methyl]benzene-1,2-diol, (II) Ersin Temel[a], Orhan Büyükgüngör[a], Mustafa Odabaşoğlu[b], Çiğdem Albayrak[b] [a]*Ondokuz Mayıs Univ., Department of Physics, Samsun-Turkey.* [b]*Ondokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.*
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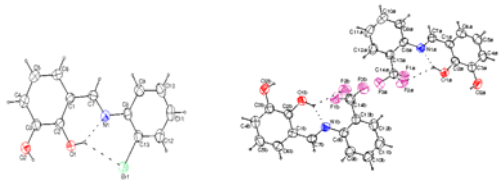
Keywords: Crystal structure; Schiff Base.

The title compounds, $C_{13}H_{10}BrNO_2$, (I), and $C_{14}H_{10}NO_2F_3$, (II), adopts the enol-imine tautomeric forms. In (I), molecule is roughly planar, with a dihedral angle of 5.13(10)° between the aromatic rings. Intra-molecular O-H...N hydrogen bonding generates an S(6) ring motif, whereas inter-molecular O-H...O hydrogen bonding links the molecules into centrosymmetric $R_2^2(10)$ dimers. In (II), molecules are nonplanar, with dihedral angles are 38.97(9) and 37.68(9)°. Each of independent molecules forms O-H...O hydrogen bonded centrosymmetric $R_2^2(10)$ dimers.



(I) (II)

MS27 P06

The NLO Properties of Organized Polymer Films: X-Ray Structure Determination of DMABI Analogs in sPMMA Andrey Tokmakov[a,b], Karlis Balodis[a], Pauls Janis Pastors[a], Sergey Belyakov[b], Inta Muzikante[c], Valdis Kampars[a], [a]*Riga Technical University, Latvia;* [b]*Latvian Institute of Organic Synthesis, Riga;* [c]*Institute of Solid State Physics of Latvian University, Riga.*
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Keywords: DMABI, X-ray structure, non-linear optical materials

2-(4'-Dimethylamino)-benzylydene-1,3-indandione (DMABI) belongs to the compounds, which exhibit non-linear optical (NLO) properties. The synthesis and study of new organic molecules possessing such properties is a subject of intense activity due to the potential application. The electro-optic characteristics of organic materials depend both from the molecular nonlinearity and morphology of the materials. If the molecular nonlinearity and properties of the materials remarkably depend on structure, the further optimization of molecular structures of DMABI analogs requests a systematic X-ray analysis. Polymer host-guest films in sPMMA (syndiotactic poly[methyl methacrylate]) containing molecules of DMABI derivatives show a different degree of NLO properties. It may arise due to different packing of the organic molecules in polymer film. The X-ray study gives the opportunity to design the models of the packing. The X-ray structures of six DMABI analogs obtained from the sPMMA polymer matrix have been determined. The packing of these compounds is characterized by stacking interactions.