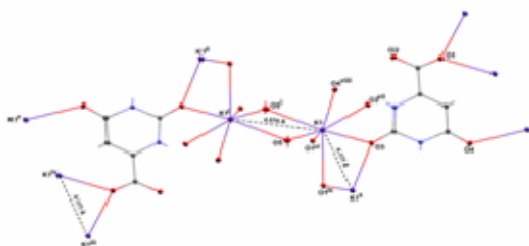
**MS15 P11**

**The novel polymeric potassium complex with a new coordination mode of orotic acid  $[K(\mu_5\text{-H}_2\text{Or})(\mu\text{-H}_2\text{O})]_n$ : Synthesis, spectral, thermal and structural characterization (H<sub>3</sub>Or = Orotic acid)**

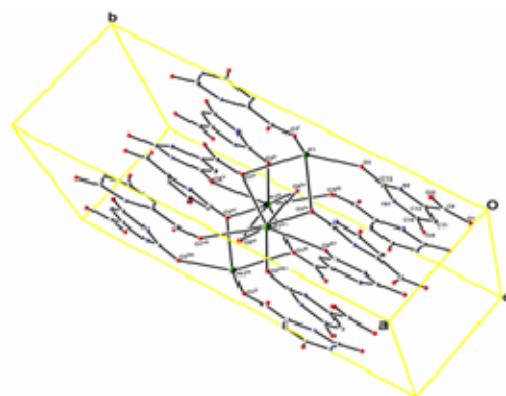
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**Keywords:** orotic acid, potassium complex, X-ray

New water and orotate bridged polynuclear seven-coordinated potassium complex,  $[K(\mu_5\text{-H}_2\text{Or})(\mu\text{-H}_2\text{O})]_n$  (H<sub>3</sub>Or = orotic acid), with unprecedented coordination mode of orotic acid has been prepared and characterized by elemental analysis, FT-IR spectra, thermal analysis (TG, DTG and DTA) techniques and X-ray diffraction. The orotate ligand exhibits new coordination mode of  $\mu_5\text{-K}(\text{O},\text{O}:\text{K}'\text{O}',\text{O}'\text{O}'')$  for H<sub>2</sub>Or<sup>-</sup> (Fig.1). The complex crystallizes in the orthorhombic space group *Pbca* with unit cell parameters:  $a = 6.524(5)$ ,  $b = 18.241(5)$ ,  $c = 12.613(2)$  Å and  $Z = 8$ . The potassium cations are seven-coordinated and are bridged by the oxygen atoms of carboxyl group, carbonyl group and aqua ligand (Fig. 2). Thermal analyses have showed decomposes in three stages over the range 20–700 °C on heating in oxygen atmosphere.



**Figure1.** The penta-dentate behaviour of the HOr ligands



**Figure2.** The coordination geometry around potassium cation and unit-cell packing.

**MS15 P12**

**Synthesis and Structural Study of  $\text{Fe}_2(\text{CO})_4[\mu_2\text{-S}(\text{CH}_2)_2\text{-S}][\text{P}(\text{OMe})_3]_2$  Complex** Abdelhamid Mousser<sup>a</sup>,

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**Keywords:** Complex, ligand, X-ray diffraction

The mononuclear or polynuclear of carbonyl metal complexes are frequently used as catalysts in organic synthesis [1] or in the preparation of other organometallic complexes [2].

Information resulting from the studies of reactivity of these complexes generally relates to the stability of the substrates under various condition reactions. The aspect more studied relates to the replacement of carbon monoxide with other ligands [3-6], their volatility makes it possible to easily eliminate them from the reactional medium.

The thermal activity of the hexacarbonyl complex  $[\mu_2\text{-S}(\text{CH}_2)_2\text{S-}]_2\text{Fe}_2(\text{CO})_6$  in the presence of an excess of trimethylphosphite  $\text{P}(\text{OMe})_3$  leads to the  $[\mu_2\text{-S}(\text{CH}_2)_2\text{S}]_2\text{Fe}_2(\text{CO})_4[\text{P}(\text{OMe})_3]_2$  complex. The spectroscopic methods confirm the disubstitution, but the provided information is insufficient to specify the regioselectivity of the exchange. The study of the regioselectivity and the stereochemistry of the replacement were realized on the basis of structural determination by X-ray diffraction. The two  $\text{P}(\text{OMe})_3$  ligands are in axial position in trans with respect to the iron-iron bond. The structure was solved on single crystal by direct methods in space group  $C_{2/c}$  and refined by least squares methods to  $R = 0.035$ .

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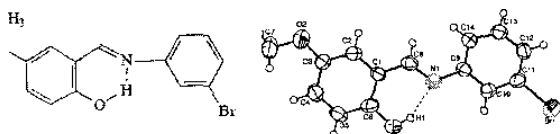
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#### MS15 P13

**Structures of Some Hydroxysalicylaldehyde Schiff Bases** Arzu Ozek<sup>a</sup>, Çigdem Albayrak, Mustafa OdabayghP, nul Odorat Büyükgüngdr' "OndoAu-Mayu Unie, Department of Physics, Samsun-Turkey. <sup>o</sup>Ondokuz Mays Univ., Department of Chemistry Samsun-Turkey  
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**Keywords:** tautomerism, hydrogen bonds, diffraction structure Analysis

The molecules of the three compounds, C<sub>14</sub>H<sub>12</sub>BrN<sub>1</sub>O<sub>2</sub> with the ortho, meta and para positions of Br (I, II and III, respectively), adopt the phenol-imine tautomeric form with strong intramolecular O-H...N hydrogen bonds.



In the compounds, the phenol-imine tautomer, is favored over the keto-amine tautomer, as indicated by the C6-O1, C8-N1, C1-C8, and C1C6 bond lengths. A similar situation was observed for 2-(3-methoxysalicylideneamino)-1H-benzimidazole monohydrate (I) - the O1-C6 bond lengths are approximately the same, indicating single-bond character, whereas the C8-N1 bond lengths are indicative of significant double bond character in (I), (II) and (III).

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#### MS15 P14

**A Preference for the Thione Structure – Lithium 2-Thiooxo-1,2-dihydropyridine-1-olate Ethanol Solvate** Ingrid Svoboda<sup>a\*</sup>, Hartmut Fuess,<sup>a</sup> Nina Schneiders, and Jens Hartung<sup>b</sup> <sup>a</sup>Department of Material Science TU Darmstadt, Germany. <sup>b</sup>Department of Organic Chemistry, Kaiserslautern, Germany.  
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**Keywords:** Thiol Thione Tautomerism, Lithium Compound, Thiohydroxamate, Pyridinethione.

2-Thiooxo-1,2-dihydropyridine-1-olate is an ambident nucleophile that is preferentially alkylated at sulfur in the presence of hard counterions, such as Na<sup>+</sup> [1]. The reactivity of the title compound, however, does not fit into this general scheme. Its inherent low reactivity toward strong electrophiles in association with a slight preference for the O-alkylation prompted us to explore its solid state structure at 300 K. Diffraction experiments performed at 100 K and 150 K surprisingly did not afford data sets of an improved quality. The compound crystallizes in P2<sub>1</sub>/c (Z = 4). Two infinite chains of Li and O give rise to Li<sub>2</sub>O<sub>2</sub> rhombi, which are tilted by approximately 90° toward one another in an accordion-like manner. Two modes of Li binding are seen in the crystal. In the first, Li is surrounded by two S- and three O-atoms leading to distorted trigonal bipyramidal coordination sphere. In the second, Li binding of four O-atoms in a distorted tetrahedral manner is seen. One corner of this tetrahedron

is occupied by an ethanol solvate molecule. The structure of the 2-thiooxo-1,2-dihydropyridine-1-olate entity of the molecule is distinctively different from the one reported for the heterocyclic cores of 2-alkylsulfanyl pyridine-1-oxides [2], bis[2-thiooxo-1,2-dihydropyridine-1-olate]nickel [3] and the corresponding zinc complex [4]. The correlation of data with those reported for N-alkoxy pyridine-2(1H)-thiones, on the other hand, fits much closer thus pointing to a preference for the thione formula of the title compound in the solid state [5].

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#### MS15 P15

**Synthesis, Structural Characterization, Electrochemical, Catalytic, Antimicrobial and Thermal Properties of the Polymeric Metal Complexes** Özlem Yılmaz<sup>a</sup>, Ertan Şahin<sup>b</sup>, Mehmet Tümer<sup>a</sup>, Mehmet Aslantas<sup>c</sup>, <sup>a</sup>Chemistry Department, Faculty of Arts and Sciences, University of KSU, 46100, Kahramanmaraş, TURKEY. <sup>b</sup>Department of Chemistry, Faculty of Arts and Sciences, Atatürk University, 25240 Erzurum, TURKEY. <sup>c</sup>Physics Department, Faculty of Arts and Sciences, University of KSU, 46100, Kahramanmaraş, Turkey.  
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**Keywords:** X-ray crystallography, electrochemical, catalytic reactions

In this study, 4-[(E)-[(4-[(1E)-(4-[(E)-[(aminophenyl)imino]methyl]phenyl)methylene]amino]phenyl)imino]methyl]benzaldehyde (L) ligand was prepared from the reaction between terephthalaldehyde with 1,4-diaminobenzene and then its metal complexes were obtained. After the oxidation reactions, in the solvent mixture, the oxidation product 3,3'-5,5'-tetra-tert-butyl-4,4'-diphenylquinone (TTBDQ) was obtained as a single crystal. The oxidation product (TTBDQ), C<sub>28</sub>H<sub>40</sub>O<sub>2</sub>, crystallizes in the space group P-1 with one-half molecule in the asymmetric unit and the other half generated by an inversion centre. The diphenylquinone moiety is planar within ±0.016(3) Å. The thermal studies for the ligand and its complexes studied. In addition, the electrochemical and antimicrobial properties of the compounds were investigated.

#### MS15 P16

**Cocrystals of oxalic acid with tricyclic quinazoline derivatives.** Akmal Tojiboev<sup>a</sup>, Kambarali Turgunov<sup>a</sup>, Bahodir Tashkhodjaev<sup>a</sup>. <sup>a</sup>S. Yunusov Institute of Chemistry of Plant Substances, Tashkent, Uzbekistan.  
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**Keywords:** crystal engineering, cocrystals, quinazoline

The design of organic solids by crystal engineering is presently of high interest [1]. Tricyclic quinazoline derivatives are potentially valuable synthons in crystal engineering: their electron donating nitrogen atom holds