

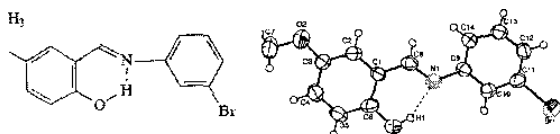
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MS15 P13

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

The molecules of the three compounds, C₁₄H₁₂BrN₁O₂ 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^{a*}, Hartmut Fuess,^a Nina Schneiders, and Jens Hartung^b ^aDepartment of Material Science TU Darmstadt, Germany. ^bDepartment 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⁺ [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 P2₁/c (Z = 4). Two infinite chains of Li and O give rise to Li₂O₂ 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^a, Ertan Şahin^b, Mehmet Tümer^a, Mehmet Aslantas^c, ^aChemistry Department, Faculty of Arts and Sciences, University of KSU, 46100, Kahramanmaraş, TURKEY. ^bDepartment of Chemistry, Faculty of Arts and Sciences, Atatürk University, 25240 Erzurum, TURKEY. ^cPhysics 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), C₂₈H₄₀O₂, 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^a, Kambarali Turgunov^a, Bahodir Tashkhodjaev^a. ^aS. 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

out the promise of different complexes with a range of electron acceptors.

Recent x-ray investigations of crystals obtained by cocrystallization of tri-, tetra- and pentamethylene-3,4-dihydroquinazolin-4-one homologues with oxalic acid shows that in the case of first two homologues cocrystal structures is formed without protonation of quinazolin-4-one molecule in the ratio 2:1, in contrast to first crystallization of pentamethylene-3,4-dihydroquinazolin-4-one with oxalic acid gives salt type crystals in the 1:1 ratio. In this case protonation occurs through nitrogen atom of quinazolone molecule and it reflects in changing of some bond lengths in the molecules of quinazoline and oxalic acid.

For comparison to first structures also the crystals of 2,3-pentamethylene-3,4-dihydroquinazolone-4 hydrochloride oxalic acid is obtained and structure is investigated.

Such research of a structure of this cocrystals of biologically active tricyclic derivatives of quinazoline [2] are important in crystal engineering terms since they offer the possibility of designing new materials through control of hydrogen bonding

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MS15 P17

On the Electronic Structure of Strong O–H···N Hydrogen Bonds [Marc Schmidtman](#)^a, Derek S Middlemiss^a, Louis J Farrugia^a, Chick C Wilson^a
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Keywords: hydrogen-bonded molecular adducts, neutron diffraction, X-ray charge density analysis

The molecular complex of isonicotinamide (IN) with oxalic acid (OA) crystallises in two polymorphic forms, with a ratio of 2:1 IN:OA. The key difference between the two polymorphs of IN₂/OA is a *cis/trans* isomerism of the OA hydroxyl. Both polymorphs share a repeating ··IN–OA–IN·· hydrogen-bonded chain motif in which short, strong hydrogen bonds (SSHBs) of the type O–H(acid)···N(pyridine) link IN and OA molecules. Enhanced covalency of the H···N bond in combination with the short O···N distance leads to an overlap of N lone-pair density with that for the H and thereby to a strong electronic delocalisation in these type of SSHBs. This makes an assignment regarding the protonation state difficult when based purely on standard X-ray crystallography. We have therefore carried out single crystal neutron diffraction and X-ray charge density studies to clarify this situation. Structural and computational results on this system will be presented.