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Keywords: MOFs, perovskites, structural analysis

MS24.P75

Acta Cryst. (2011) A**67,** C386

Novel amidrazone derivative and its Cu(II) complex: Crystal structure and antitumor activity

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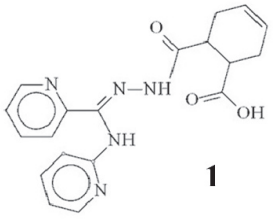
Compounds with an open chain amidrazone system, N–C=N–N, (Scheme) constitute a unique group of ligands with their propen-sity to react with a wide range of transition metals in their neutral or ionic forms as well as diversity of their coordination modes [1]. Depending on the quality of the metal center and experimental conditions they can form mono-, bi- and poly-nuclear species. These properties make them useful in design and synthesis of novel functional materials. However, the most extensive studies of hydrazones are related to their pharmacological properties. It has been shown that some of them exhibit significant antibacterial and antitumor properties [2], [3].

X-ray diffraction analysis of 6-acetyl-cyclohex-3-enecarboxylic acid [1-pyridin-2-yl-1-(pyridyn-2-yloamin)meth-(Z)-ylidene] hydrazide, H_2L, (1) and its copper(II) complex $[Cu_2L_2]\cdot 4H_2O$ (2) has been carried out in order to elucidate the influence of coordination and amide protonation state on the geometry of the ligand.



1

H_2L (1)	$[Cu_2L_2]\cdot 4H_2O$ (2)
$P2_1/n$	$P2_1/c$
a = 10.769(2) Å	a = 9.979(1) Å
b = 11.423(1) Å	b = 21.406(2) Å
c = 14.628(2) Å	c = 9.046(1) Å
β = 99.45(1)°	β = 103.39(1)°
V = 1775.0(4) Å^3	V = 1879.8(3) Å^3
Z = 4	Z = 2
R_1 = 0.0511	R_1 = 0.0484

Structural analysis shown that compound (1) exists in his amide-hydrazone form in the solid state. The central amidrazone moiety has a Z configuration with respect to the hydrazone C=N double bond. The N^3–C^2=N^2–N^1–(C^1=O^1) chain, which adopts a cis,trans,cis conformation, is almost planar. All atoms of the acylamidrazone moiety may be regarded as sp^2 hybridized. Near-planarity of this unit may suggest a high level of π-electron delocalization. However, the X-ray data indicate, that there is a clear distinction between single and double bonds in this part of molecule.

The reaction of H_2L (1) with copper(II) acetate results in double deprotonation of the ligand, namely the carboxylic and amide groups. This induces considerable π-electron delocalization along the whole acylamidrazone system. Furthermore, the ligand configuration is found to be transferred from Z to E upon metal complexation. The elementary building units in crystal (2) are centrosymmetric binuclear species. Isomerization around the C=N bond allows the L^{2-} ions to chelate the Cu^{2+} ion through its pyridine-N, amide-O and imine- N atoms. The carboxylate O atom from the adjacent, inversion-related ligand completes the square-planar donor arrangement around the metal center.

In cytotoxicity research, (2) shown a high in vitro cytotoxic properties against SW 948, CX-1 and A-431 cancer cell lines, whereas growth inhibition activity of the free ligand (1) was no significant.

This work was supported by the Polish Ministry of Science and Higher Education (project No. N204 546839).

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Keywords: amidrazone, copper complex, crystal structure

MS24.P76

Acta Cryst. (2011) A**67,** C386-C387

Molecular imprinting effect of the guest in β-cyclodextrin inclusion complexes

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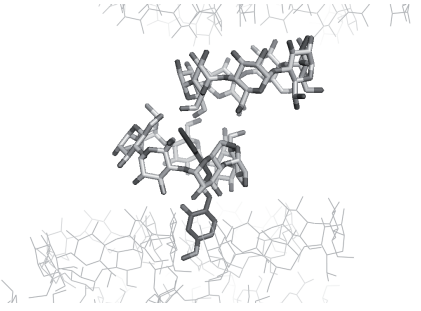
Cyclodextrins (CDs) are well known, water soluble, cyclic oligosaccharides, which are used for micro encapsulation of organic molecules inside their relatively apolar cavity. βCD inclusion complexes of two Schiff bases (anils), derivatives of salicylideneaniline, changed the behaviour of the anils from thermochromic (as free crystalline compounds) to photochromic upon encapsulation [1]. Trials to grow single crystals of the βCD/anil complexes from absolute ethanol resulted in isomorphous crystals (P21, a=15.887(8), b=14.784(12), c=15.29.680 (14) Å, β=103.19(2)°, Z=2) exhibiting a novel packing, observed for the first time, accompanied by dramatic distortions of the βCD conformations. Refinement of both structures did not reveal the guest in a clearly detectable amount, the structures appearing as *β*CD-ethanol complexes. However, they differ also from any of the three known forms, I – III, of βCD/ethanol complexes [2]. The structures exhibit an open space at the secondary entrance of one of the host monomers, in which the hydrophilic salicylidene moiety of the guests can fit (Figure). It is proposed that the βCD/anil complexes were initially formed by inclusion of the hydrophobic-half of the guests inside the host cavity and the salicylidene part extending outside the entrance of the secondary face. Subsequently, the anils were solvolysed thereby emptying the cavity and lattice. However due to the low solubility of βCD in ethanol, the formed crystals remained intact bearing the molecular imprint of the guest, whereas its place in the crystals has been taken eventually by ethanol molecules.



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