In this work, we have used (NH₃)₂[PtCl₆]x[ReCl₆]1-x as the precursor because of the ability to form double complex salts with a required metal composition. The compounds (NH₃)₂[PtCl₆][ReCl₆]₁ₓ (x = 0.40(I), 0.50(II), 0.60(III)) have been synthesized by adding NH₃Cl to aqueous solutions of K₂[PtCl₆][ReCl₆]₁ₓ. The latter have been obtained by mixing aqueous solutions of the isostructural complex salts K₂[PtCl₆] and K₂[ReCl₆] in required quantities. Thermal decomposition of the title compounds has been studied. The prepared solid solutions have been characterized by X-ray electron spectroscopy. It shows the pseudomorphism of the crystals of double complex salts. The final products of thermal decomposition are different for each precursor and depend on the initial metal proportions. Compounds II and III decompose to yield two phases. One of them is a solid solution based on the platinum cell and the other is the metal rhenium. Thermal decomposition of I gives a solid solution based on the rhenium cell with the parameters similar to the initial metal proportion. The work has been supported by RFBR Grant 03-08-00603 and Presidium SB RAS interdisciplinary project No 112.

Keywords: platinum compounds; solid solutions; thermal decomposition

FA4-MS06-P18

Copper (II) Risedronate: the Importance of Structure Validation on the Correct Solution. Miriam Rossi,a Bruno Demoro,a Lucia Otero,a Dinorah Gambino,a Francesco Caruso,b "Department of Chemistry, Vassar College, Poughkeepsie, NY, 12604, USA. bCatedra de Quimica Inorganica, Facultad de Quimica, UDELAR, 11800 Montevideo, Uruguay. cIstituto di Chimica Biomolecolare, CNR, c/o Universita di Roma “La Sapienza” Ple. Aldo Mora5, 00185, Rome, Italy.
E-mail: rossi@vassar.edu

Chagas’ disease (American Trypanosomiasis) is a major cause of death and hardship in the impoverished regions of the developing world. It is the largest parasitic disease burden in the American continent being endemic in 21 countries from southern United States to Argentina and Chile. Our preliminary results show that sodium risedronate has activity against Chagas’ disease; therefore, interest in developing effective drugs against this disease has led to using risedronic acid and sodium risedronate (Actonel) as ligands in metal complexes. These compounds are bisphosphonates used to strengthen bone, for osteoporosis, and Paget’s disease. In this meeting, we present the crystal structure of copper(II) risedronate.

The paramagnetic nature of the Cu(II) metal precluded NMR spectra from being collected and the chemical composition analysis, for C, H and N content, could not provide absolute certainty of crystal composition. For instance, the sodium ion and water hydrate composition could not be a priori defined. From our data, we were able to obtain 2 potential structural solutions. One had the copper (II) complex and included Na ions; it had a satisfactory R₀ of 0.0538 (Rw 0.0561) although some structural features appeared suspicious.

In the other, we replaced the Na⁺ by a water oxygen, and obtained an R₀ of 0.0253 (Rw 0.0282), with satisfactory geometrical, structural and intermolecular interactions showing it to be the real structure.

In this poster, we wish to address the problem of interpreting reasonable looking, but wrong, structures. What parameters are best used in judging the correctness of a crystal structure? Crystallographers have grappled with this issue [1], [2] and PLATON and CIF validation methods are highly useful. However, we wonder about structures deposited in the CSD having R₀ even larger than 5%, are all of them correct?


Keywords: coordination crystal chemistry; copper (II) coordination complexes; structure validation

FA4-MS06-P19

Synthesis and Crystal Structure of [Fe(II) (L)]ClCH₂CH₂OH·2H₂O (H₂L=Pyridoxal-semicarbazone). Violeta S. Jevtovic. University of Novi Sad, Faculty of Sciences, Department of Chemistry, Novi Sad, Serbia. Stevan Jankov; University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Serbia.

E-mail: Violeta@ih.ns.ac.yu

Brown single crystals of the title compound C₁₆H₁₆ClFeN₅O₅ wer prepared by reaction of MeOH solutions of FeCl₃·6H₂O and H₂L·H₂O in mole ratio 1:2. The complex has octahedral
configuration with two non-equivalent tridentate ligands with O,N,O donors: one of the ligands having deprotonated semicarbazido fragment, whereas for the other additional deprotonation involves the pyridine nitrogen. The compound crystallizes in the P-1 space group with \( a = 8.7273(3) \text{ Å} \), \( b = 12.3030(4) \text{ Å} \), \( c = 14.3589(6) \text{ Å} \), \( α = 109.118(3) \), \( β = 100.490(3) \), \( γ = 101.860(3) \), \( V = 1372.79 \text{ Å}^3 \).

The formation of \( \text{Pb(Zr, Ti)}_3 \text{O}_9 \) precursor powders of high homogeneity of components. Temperature processing ceramic fabrication demands fine ceramic at a temperature as low possible. Low firing poor microstructure because of the high-temperature such as nonstoichiometry, compositional fluctuation and solid-state reaction. However, there are undesirable features etc [1]. In general, the PZT are processed by the traditional electronic buzzers and ringers, pressure and stress sensors, materials often used in ultrasonic generators, hydrophones, etc [1].

In designing these polymers the properties of linking ligands in determining the structural outcomes of target polymers. The relative orientation of donor atoms obey a fundamental role such as various coordination modes, variable lengths and the effects of calcination temperature on lattice parameters and tetragonality of PZT powders have been discussed, differential thermal analysis (DTA) and thermal gravimetric analysis (TGA).

The formation of PZT is accomplished through several steps: decomposition of \( \text{PbO} \rightarrow \text{Pb} \), formation of \( \text{PbTiO}_3 \) solid solution at 600°C above 400°C and of its solid solution at 600°C.


Keywords: PZT; RX; thermal properties

FA4-MS06-P21

Crystal Structure of Bipyridine Type Ligand \( \text{L} = \text{N}, \text{N}-\text{bis-pyridin-2-ylmethylene-naphthalene-1,5-diamine,} \text{Niloofar Akbarzadeh.} \)

The current interest in the crystal engineering of polymeric coordination networks stems from their potential applications as zeolite like materials for molecular selection, ion exchange and catalysis as well as in the variety of architectures and topologies [1–2]. One of the basic strategies for crystal engineering utilizes metal-ligand bonding between transition metals and organic ligands to create coordination polymers.

In designing these polymers the properties of linking ligands such as various coordination modes, variable lengths and relative orientation of donor atoms obey a fundamental role in determining the structural outcomes of target polymers. A novel bipyridine-type linking ligand \( \text{L} = ((\text{2-py})-\text{CH} = \text{N}-\text{C}_6\text{H}_4\text{N}-(\text{CH} = \text{N}-(\text{2-py})) \) (Fig. 1) was prepared by the Schiff-base condensation and fully characterized by spectroscopic methods and single-crystal X-ray diffraction. The unit cell parameters are: space group \( \text{P21/c with a = 4.8666(8) Å, b} \)