the intralayer Mn-Mn distance. The magnetic ordering of the Mn layers along the c-axis is antiferromagnetic for the smaller value than the critical intralayer Mn-Mn distance or ferromagnetic for the bigger that value [1 and the references therein]. Since the intralayer Mn-Mn distance of the SmMn$_x$Ge$_{2-x}$ compounds is very close to the critical distance, the multiple magnetic phase transitions are observed as a function of the temperature. Because of the multiple magnetic phase transitions, this compound is very good candidate to investigate the magnetoresistance and magnetocaloric effect.

SmMn$_{0.05}$Ge$_{1.95}$ (x=0.05 and 0.1) and SmMn$_{0.05}$Co$_{0.95}$Ge$_{2}$ (x=0.05 and 0.15) compounds are prepared by using arc melting under argon atmosphere. All compounds crystallize in ThCr$_2$Si$_2$-type tetragonal structure. The temperature and magnetic field dependence of magnetization are measured in an applied field up to 5 T between 10 and 350 K. The magnetocaloric effect-MCE is calculated by using Maxwell’s relation and Landau theory. Both calculated MCE values are good accordance. For the SmMn$_{0.05}$Fe$_{0.95}$Ge$_2$ and SmMn$_{0.05}$Co$_{0.95}$Ge$_2$ compounds, the positive and negative MCE are observed. Resistivity measurements are performed by a four probe method as function of the temperature (between 70 and 350K) and magnetic field (up to 7 T). The magnetoresistance effect is also observed at the magnetocaloric transition. At T$_c$, the magnetoresistance effect $\Delta \rho/\rho$ is about -%20 and -%12, respectively.


Keywords: magnetoresistance effect; magnetocaloric effect; magnetic measurements

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Structure-magnetism Relationship in Mononuclear Co(II) Complexes. Blažena Papánková, Roman Boča, Lubor Dilháň, Ingrid Svoboda, Hartmut Fuess. *Institute of Inorganic Chemistry (FCHPT), Slovak University of Technology, 812 37 Bratislava, Slovakia. 1Institut for Materials Science, Darmstadt University of Technology, 64289 Darmstadt, Germany.
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Structure-magnetism relationship represents a long-lasting trend in the coordination chemistry. It is manifested by a number of magnetostuctural J-correlations where the exchange coupling constant (J) is correlated with some structural parameters (bond angles in bridged complexes). Recently, a magnetostuctural D-correlation has been proposed for Ni(II) complexes [1]. Within this contribution, a series of mononuclear Co(II) complexes has been synthesized and structurally characterized with the aim to correlate the zero-field splitting parameter (D) with the structural tetragonality of cobalt complexes.


Keywords: magnetic properties; cobalt compounds; structure correlation

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Liquid crystals containing metal are called metallomesogens. It is a great interest to develop the metallomesogens because it is expected to show interesting physical properties such as electrical, magnetic and so on in addition to liquid crystallinity. The liquid crystalline ferrocene derivatives are one of the metallomesogens. The structure of liquid crystalline phase may depend on that of crystal one. Therefore, it is important to analyze the crystal structure in order to understand the phase transition mechanism.

In our laboratory, many structural studies on liquid crystalline 1,1’-di-substituted ferrocene derivatives have been performed. The results obtained reveal three different crystal types, “S” shaped [1], “U” shaped [2] and “Z” shaped [3] structures. Recently, structure analysis of liquid crystalline mono-substituted ferrocene derivatives, of which substituent is the same as that of the 1,1’-di-substituted ferrocene ones, has carried out. The result obtained shows that it is closely resemble in the half of the structure of 1,1’-di-substituted ferrocene derivatives already analyzed [4]. In this study, the crystal structures of many other liquid crystalline mono-substituted ferrocene derivatives are determined by X-ray structure analysis. Using these results, correlation of the structures of 1,1’-di-substituted ferrocene derivatives with those of mono-substituted ones are discussed.


Keywords: ferrocene compounds; liquid-crystal structures; X-ray structure analysis

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Crystallographic Analysis of Pr-Re System. Elena Shusharina, Andrey Zadesenets, Sergey Gromilov. *Faculty of Natural Science, Novosibirsk State University, Russia. 1Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia.
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Platinum and rhenium–platinum solid solutions are used as effective catalysts in petrol reforming. The synthesis of such compounds by using double complex salts as precursors is widely applied. A Pt-Re phase diagram belongs to the peritectic type, the two-phase region at
T = 800 °C being limited with Pt0.60Re0.40 and Pt0.67Re0.33 compositions [1]. Figure shows the correlation between V/Z and the composition for all known reference materials. The Pt0.60Re0.40–Pt0.33Re0.67 interval is unusual because of the V/Z value which is lower than that for pure rhenium. The solid solutions Re0.75Pt0.25 and Re0.67Pt0.33 have been obtained by thermal decomposition of [Pt(NH3)4]2(ReO4)2 and [Pt(NH3)4Cl2](ReO4)2·2H2O [2, 3].

In the present work, we have used (NH3)4[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)4[PtCl6]x[ReCl6]1-x (x = 0.40(I), 0.50(II), 0.60(III)) have been synthesized by adding NH4Cl to aqueous solutions of K3[PtCl6]·xH2O. The latter have been obtained by mixing aqueous solutions of the isostructural complex salts K3[PtCl6] and K3[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 with the parameters a = 12.606(2) Å, b = 15.209(3) Å, c = 15.289(3) Å, β = 92.47(2)°. 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.

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Keywords: platinum compounds; solid solutions; thermal decomposition

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Copper (II) Risedronate: the Importance of Structure Validation on the Correct Solution. Miriam Rossi1, Bruno Demoro2, Lucia Otero3, Dinorah Gambino4, Francesco Caruso4, 1Department of Chemistry, Vassar College, Poughkeepsie, NY, 12604, USA. 2Catedra de Quimica Inorganica, Facultad de Quimica, UDELAR, 11800 Montevideo, Uruguay. 3Istituto di Chimica Biomolecolare, CNR, c/o Universita di Roma “La Sapienza” Ple. Aldo Moro5, 00185,Rome, Italy.
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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 Rf 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 Rf 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 R even larger than 5%, are all of them correct?


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

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Synthesis and Crystal Structure of [Fe(II)(L)(Cl)×3(CICH2CH2OH)2·2H2O (H,L=Pyridoxal-semicarbazone). Violeta S. Jevtovic. University of Novi Sad, Faculty of Sciences, Department of Chemistry, NoviSad, Serbia.Stevan Jankov; University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Serbia.
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Brown single crystals of the title compound C12H13ClFeN2O5 were prepared by reaction of MeOH solutions of FeCl3·6H2O and H2L·H2O in mole ratio 1:2. The complex has octahedral...