

the intralayer Mn-Mn distance. The magnetic ordering of the Mn layers along the c-axis is antiferromagnetic for the smaller value than the critic intralayer Mn-Mn distance or ferromagnetic for the bigger than that value [1 and the references therein]. Since the intralayer Mn-Mn distance of the SmMn_2Ge_2 compounds is very close to the critic 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.

$\text{SmMn}_{2-x}\text{Fe}_x\text{Ge}_2$ ($x=0.05$ and 0.1) and $\text{SmMn}_{2-x}\text{Co}_x\text{Ge}_2$ ($x=0.05$ and 0.15) compounds are prepared by using arc melting under argon atmosphere. All compounds crystallize in ThCr_2Si_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 $\text{SmMn}_{1.95}\text{Fe}_{0.05}\text{Ge}_2$ and $\text{SmMn}_{1.85}\text{Co}_{0.15}\text{Ge}_2$ compounds, the positive and negative MCE are observed. Resistivity measurements are performed by a four probe method as function of temperature (between 70 and 350K) and magnetic field (up to 7 T). The magnetoresistance effect is also observed at the metamagnetic transition. At T_c^{sm} , the magnetoresistance effect $\Delta\rho/\rho$ is about -%20 and -%12, respectively.

[1] Dincer, I.; Elmali, A.; Elerman, Y.; *J. Magn. Magn. Mater.*, **2004**, 271, 348.

Keywords: magnetoresistance effect; magnetocaloric effect; magnetic measurements

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Structure-magnetism Relationship in Mononuclear Co(II) Complexes. Blažena Papánková^a, Roman Boča^a, Lubor Dlháň^a, Ingrid Svoboda^b, Hartmut Fuess^b. ^a*Institute of Inorganic Chemistry (FCHPT), Slovak University of Technology, 812 37 Bratislava, Slovakia.* ^b*Institut für Material Science, Darmstadt University of Technology, 64289 Darmstadt, Germany.*

E-mail: blazena.papankova@stuba.sk

Structure-magnetism relationship represents a long-lasting trend in the coordination chemistry. It is manifested by a number of magnetostructural J-correlations where the exchange coupling constant (J) is correlated with some structural parameters (bond angles in bridged complexes). Recently, a magnetostructural 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.

[1] Boča, R.; Titiš, J. „Magnetostructural D-Correlation for Zero-Field Splitting in Nickel(II) Complexes“ in *Coordination Chemistry Research Progress*, Nova Science Publishers, New York, **2007**, pp.247-304

Keywords: magnetic properties; cobalt compounds; structure correlation

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Structure of Liquid Crystalline Mono-substituted Ferrocene Derivatives. Naotake Nakamura^a, Kazuya Hiro^a, Kenjiro Uno^a. ^a*Department of Applied Chemistry, Ritsumeikan University, Kusatsu, Shiga, Japan.*

E-mail: nakamura@sk.ritsumei.ac.jp

Liquid crystals containing metal are called metallomesogen. 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.

[1] Nakamura N., Okabe T., Takahashi T., *Mol.Cryst.Liq.Cryst.*, **2002**, 383, 27. [2] Okabe T., Nakazaki K., Igaue T., Nakamura N., Donnio B., Guillon D., Gallani J.-L., *J.Appl.Cryst.*, **2009**, 42, 63. [3] Nakamura N., Nishikawa M., *Chem.Lett.*, **2005**, 34, 1544. [4] Nakamura N., Hiro K., Nishikawa M., Okabe T., Uno K., *Mol. Cryst.Liq. Cryst.*, to be submitted.

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

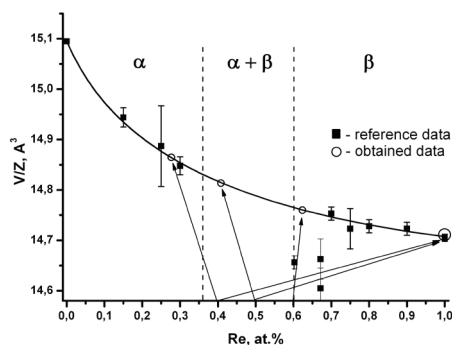
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Crystallochemical Analysis of Pt-Re System. Elena Shusharina^a, Andrey Zadesenets^b, Sergey Gromilov^b. ^a*Faculty of Natural Science, Novosibirsk State University, Russia.* ^b*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia.*

E-mail: knilav@ngs.ru

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 $\text{Pt}_{0.64}\text{Re}_{0.36}$ and $\text{Pt}_{0.40}\text{Re}_{0.60}$ compositions [1]. Figure shows the correlation between V/Z and the composition for all known reference materials. The $\text{Pt}_{0.40}\text{Re}_{0.60}$ – $\text{Pt}_{0.33}\text{Re}_{0.67}$ interval is unusual because of the V/Z value which is lower than that for pure rhenium. The solid solutions $\text{Re}_{0.67}\text{Pt}_{0.33}$ and $\text{Re}_{0.75}\text{Pt}_{0.25}$ have been obtained by thermal decomposition of $[\text{Pt}(\text{NH}_3)_4](\text{ReO}_4)_2$ and $[\text{Pt}(\text{NH}_3)_3\text{Cl}](\text{ReO}_4)_3 \cdot 2\text{H}_2\text{O}$ [2,3].



In the present work, we have used $(\text{NH}_4)_2[\text{PtCl}_6][\text{ReCl}_6]_{1-x}$ as the precursor because of the ability to form double complex salts with a required metal composition. The compounds $(\text{NH}_4)_2[\text{PtCl}_6][\text{ReCl}_6]_{1-x}$ ($x = 0.40$ (I), 0.50 (II), 0.60 (III)) have been synthesized by adding NH_4Cl to aqueous solutions of $\text{K}_2[\text{PtCl}_6][\text{ReCl}_6]_{1-x}$. The latter have been obtained by mixing aqueous solutions of the isostructural complex salts $\text{K}_2[\text{PtCl}_6]$ and $\text{K}_2[\text{ReCl}_6]$ 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.

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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^b, Lucia Otero^b, Dinorah Gambino^b, Francesco Caruso^c. ^aDepartment 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 Moro5, 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 R_f 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 R_f 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_f even larger than 5%, are all of them correct?

[1] Spek, A.L. *J. Appl. Cryst.* **2003**, 36, 7. [2] Spek, A.L. *Acta Cryst.* **2009**, D65, 148.

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

FA4-MS06-P19

Synthesis and Crystal Structure of $[\text{Fe}(\text{HL})(\text{L})]\text{Cl} \cdot \text{CH}_3\text{CH}_2\text{OH} \cdot 2\text{H}_2\text{O}$ ($\text{H}_2\text{L} = \text{Pyridoxal-semicarbazone}$). 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 $\text{C}_{20}\text{H}_{31}\text{ClFeN}_8\text{O}_9$, were prepared by reaction of MeOH solutions of $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ and $\text{H}_2\text{L} \cdot \text{H}_2\text{O}$ in mole ratio 1:2. The complex has octahedral