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Keywords: platinum group; X-ray powder diffraction; crystal structure analysis

FA4-MS06-P12

Heterobimetallic Malonate-Containing Molecular Compounds. Laura Cañadillas-Delgado^a, Fernando S. Delgado-Trujillo^b, Óscar Fabelo^a, Jorge Pasán^a, Javier Campo-Ruiz^c, Garry McIntyre^d, Yolanda Rodríguez-Martín^a, Catalina Ruiz-Pérez^a. ^aLaboratorio de Rayos X y Materiales Moleculares, Dpto. de Física Fundamental II, Fac. Física, Avda. Astrofísico Fco. Sánchez,s/n. La Laguna, S/C de Tenerife. Spain. ^bBM16-LLS european Synchrotron Radiation Facility, 6 Rue Jules Horowitz-BP 220, 38043 Grenoble Cedex 9, France. ^cInstituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, C/ Pedro Cerbuna 12, Zaragoza. Spain. ^dInstitut Laue Langevin, 38100, Grenoble, France. E-mail: Idelgado@ull.es

There has been an increasing interest in complexes containing paramagnetic metal ions exhibiting extended networks because of their potential applications in molecular magnetic materials [1]. In the context of our magneto-structural research with malonate-containing complexes with first-row metal transition centres, we have characterized the homometallic malonate-containing compounds of formula $[M(H_2O)][M(mal)_2(H_2O)_2]$ [M = Co(II), Ni(II) and Zn(II)]. They crystallize in a monoclinic structure with space group C2/m, the metal atoms lying on a 2/m site [2].

In these context we have synthesized three new heterobimetallic compounds of formula $[M_xM'_{1-x}(H_2O)]$ $[M_yM'_{1-y}(mal)_2(H_2O)_2]$, which are isostructural with the malonate-containing homometallic complexes, previously studied.

A quantitative analysis of a crystal of each sample through the X-ray microanalysis technique by using a copper pattern have been made, the analysis showing that M and M' ions are present in a 1:1 molar ratio. The single crystal X-ray studies don't allow us to distinguish each metal ion, due to the similar form factor, and therefore different crystal structures are possible; alternation of the homometallic layers or existence heterometallic planes within the crystal structure.

The aim of a proposed neutron diffraction experiment was, therefore, to determine the cationic distribution of the metal atoms in the crystal structure (Laue diffractometer VIVALDI).

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Keywords: neutron diffraction techniques; bimetallics; carboxylic acids

FA4-MS06-P13

Syntheses and Crystal Structures of Two New Tricoordinate Cu(I) Complexes with Bidentate Schiff Base Ligands. <u>Hadi Kargar</u>^a, Reza Kia^b, Hoong-Kun Fun^b. ^aDepartment of Chemistry, School of Science, Payame Noor University (PNU), Ardakan, Yazd, Iran. ^bX-ray Crystallography Lab., School of Physics, Universiti Sains Malaysia, 11800, Penang, Malaysia.

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The coordination chemistry of copper(I) complexes has received increased attention over the last decades. This is mainly due to the potential application of these complexes in catalytic processes, photosensitization reactions, lightharvesting studies, and the design of supramolecular arrays [1,2]. The steric, electronic, and conformational effects imparted by the coordinated ligands play an important role in modifying the properties of the prepared metal complexes. In recent years, an increasing amount of research has been focused on the design and preparation of mono or dinuclear mixed ligand transition metal complexes with neutral, chelating nitrogen-containing ligands [3]. Here we report the crystal structures of two new tricoordinate Cu(I) complexes with two bidentate Schiff base ligands and copper(I) iodode. To the best of our knowledge, these complexes are the first tricoordinate complexes of copper(I) iodide with two bidentate unconjugated Schiff base ligands.

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Keywords: copper(I) complexes; schiff base; bidentate ligand

FA4-MS06-P14

Magnetoresistance and Magnetocaloric Effect of the SmMn_{2-x}T_xGe₂ (T:Fe and Co; x=0.05, 0.1 nd 0.15) Compound. <u>Yalcin Elerman</u>^a, Ilker Dincer^a, Guliz Sevgül^a. ^aDepartment of Engineering Physics, Ankara University, Ankara Turkey. E-mail: <u>elerman@ankara.edu.tr</u>

During past three decades, extensive investigations have been performed on magnetism of the intermetallic compounds RMn_2X_2 (R: rare earth, X: Si or Ge) which are characterized by a layered arrangement of R, Mn and X atoms. The magnetic properties of these compounds are governed by 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 SmMn₂Ge₂ 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.

SmMn_{2-x}Fe_xGe₂ (x=0.05 and 0.1) and SmMn_{2-x}Co_xGe₂ (x=0.05 and 0.15) compounds are prepared by using arc melting under argon atmosphere. All compounds crystallize in ThCr₂Si₂-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_{1.95}Fe_{0.05}Ge₂ and SmMn_{1.85}Co_{0.15}Ge₂ 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_cSm, the magnetoresistance effect $\Delta \rho/\rho$ is about -%20 and -%12, respectively.

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Keywords: magnetoresistance effect; magnetocaloric effect; magnetic measurements

FA4-MS06-P15

Structure-magnetism Relationship in Mononuclear Co(II) Complexes. <u>Blažena Papánková</u>^a, Roman Boča^a, Ľubor Dlháň^a, Ingrid Svoboda^b, Hartmut Fuess^b. *aInstitute of Inorganic Chemistry (FCHPT), Slovak University of Technology, 812 37 Bratislava, Slovakia. bInstitut 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 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

FA4-MS06-P16

Structure of Liquid Crystalline Mono-substituted Ferrocene Derivatives. <u>Naotake Nakamura</u>^a, Kazuya Hiro^a, Kenjiro Uno^a. ^aDepartment of Applied Chemistry, Ritsumeikan University. Kusatsu, Shiga, Japan.

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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.

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

FA4-MS06-P17

Crystallochemical Analysis of Pt-Re System. <u>Elena</u> <u>Shusharina</u>^a, Andrey Zadesenets^b, Sergey Gromilov^b. ^aFaculty of Natural Science, Novosibirsk State University, Russia. ^bNikolaev 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

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