

$V=1437.7(3)\text{\AA}^3$; $Z=2$ for (2). The copper(II) ions present a square base pyramidal geometry in these reported complexes with a Cu-Cu distance of 5.013 and 5.017 Å for (1) and (2) respectively. Both compounds present antiferromagnetic behaviour with T_m of 15.5 and 32 K for (1) and (2). The magnetic behaviour will be compared with other reported Cu-VPO systems.¹

Acknowledgements: FONDAP 11980002, ECOS-CONICYT C02E01 Grants.

[1] Moreno Y., Vega A., Ushak S., Baggio R., Peña O., Le Fur E., Pivan J.Y., Spodine E., *J. Mater. Chem.*, 2003, **13**, 2381.

Keywords: magnetic materials, copper, VPO system

P.08.14.6

Acta Cryst. (2005). A61, C342

Partial Phase Diagram of Pd-Mn System Studied by Electron Diffraction and Microscopy

Rokuro Miida, Tokyo University of Science, Suwa, Chino Nagano, Japan. E-mail: miida@rs.suwa.tus.ac.jp

Among ordered phases reported in the present alloy system, four of Pd₃Mn (or Pd₃Mn II), Pd₂Mn, Pd₅Mn₃ and PdMn were confirmed to be stable, but no indications of Pd₃Mn I and Pd₂₁Mn₁₁ were obtained.

In the solid solution range from 25 to 50at%Mn, the crystal structure continuously transforms from D0₂₃ type to L1₀ type with increasing Mn content. The magnitude of c_0/a_0 of the basal lattice is 1.0 for 25.0-26.5at%Mn, and then decreases down to 0.91 at 36.1at%Mn. The Pd₃Mn phase is defined in the range from 25.0 to 26.5at%Mn, because $c_0/a_0=1.0$ in this range is the characteristic of D0₂₃ type structure. The electron micrograph shows the arrangement of minority atoms (Mn) in D0₂₃ type. For Mn content more than 37at%, the PdMn phase with L1₀ type is stable above 600°C. In the compositions between Pd₃Mn and PdMn phases, the occupation probability of Mn at each atom-site was expressed in terms of alloy composition.

The Pd₂Mn phase is stable below 700°C. The electron micrograph shows the arrangement of Mn atoms, which supports the structural model reported already [1]. The Pd₅Mn₃ phase was confirmed by electron diffraction patterns with different incidences. This phase is ranked as the second ordered structure of the PdMn phase. On the basis of ordered structures confirmed there, a partial phase diagram was proposed for Pd-rich Pd-Mn alloys.

[1] Kádár G., Krén E., Márton M., *J. Phys. Chem. Solids*, 1972, **33**, 212.

Keywords: electron diffraction, ordered structures, phase diagrams

P.08.14.7

Acta Cryst. (2005). A61, C342

Crystal Structure of β -KU₂(PO₄)₃ – a Member of the Group with NZP Structure Type

Elena Gobecheva^a, Yuri Kabalov^a, Sergei Tomilin^b, Anatolii Lukinikh^b, Andrei Lizin^b, ^aFaculty of Geology, Moscow State University, Russia. ^bFederal State Unitary Enterprise «State Scientific Center Of Russian Federation –Research Institute Of Atomic Reactors», Dimitrovgrad, Russia. E-mail: elglob@mail.ru

The study of synthetic double Potassium-Uranium orthophosphate KU₂(PO₄)₃ is part of a program on the crystal chemistry of double orthophosphates with general formula (M1)_{0→1}(M2)_{0→3}{[L₂(PO₄)₃]^P}_{3z}, where (M1)_{0→1} and (M2)_{0→3} are types of extraframework cation positions in holes with the indications of position numbers and L is the framework position, that includes determination of phases obtained by sol-gel technique. The NaZr₂(PO₄)₃ (NZP) structural type [1] is widely distributed among them. The distinguishing characteristic feature of the NZP structure is that the same crystallographic positions in this structure can accommodate elements, both small and large, in oxidation states from +1 to +5 with retention of the principal framework. In this work the compound β -KU₂(PO₄)₃ was recently studied by x-ray powder diffraction and Rietved method in space group R-3c. The synthesis of new framework phosphates belonging to

the NZP structural type, as well as detailed analysis of the geometric and topological features of the structures of new and known NZP-type phosphates aimed at revealing correlations between the crystal structures of these compounds and the practically valuable physicochemical properties, have attracted considerable attention in recent years [2].

[1] Hong H.Y.-P., *Mat. Res. Bull.*, 1976, **11**(2), 173-182. [2] Alamo J., *Solid State Ionics.*, 1993, **63-65**, 547.

Keywords: phosphates, X-ray diffraction, Rietveld method

P.08.14.8

Acta Cryst. (2005). A61, C342

Transition Metal Hydroxy-Terephthalates: Structure-Magnetism Relationship

Anne Carton^a, Michel François^a, Pierre Rabu^b, ^aLCSM, University H.Poincaré, Nancy, France. ^bIPCMS UMR7504 CNRS-ULP, Strasbourg, France. E-mail: anne.carton@lcsm.uhp-nancy.fr

The title compounds belong to the family of hybrid lamellar materials where transition metal ions form layers spaced by organic anions. Metal hydroxy-terephthalates M_x(OH)_{2x-2}(tp) (tp =C₈H₄O₄, M = Zn, Mn, Fe, Co, Ni, Cu) have been synthesized by hydrothermal route and their crystallographic structures were determined. Zn₃(OH)₄(tp) has been characterized from X-ray single crystal diffraction data: C2/c, $a=28.100\text{\AA}$, $b=6.310\text{\AA}$, $c=14.836\text{\AA}$, $\beta=121.56^\circ$. The zinc atoms exhibit tetrahedral, octahedral and bi pyramidal coordinations, forming step-like layers bridged by terephthalate moieties. As for the paramagnetic ions, the layered structures of the model compounds Co₂(OH)₂(tp) (C2/m, $a=19.943\text{\AA}$, $b=3.289\text{\AA}$, $c=6.289\text{\AA}$, $\beta=95.75^\circ$) [1] and Cu₂(OH)₂(tp) (P-1, $a=10.143\text{\AA}$, $b=6.339\text{\AA}$, $c=3.484\text{\AA}$, $\alpha=99.17^\circ$, $\beta=95.75^\circ$, $\gamma=98.76^\circ$)[2] were determined *ab-initio* from XRPD data. The metallic cations lie in oxygen octahedra. Despite similar structures, different magnetic behaviors are observed depending on the metal ion and on symmetry differences. Low-temperature ferromagnetic-like ordering will be discussed on the basis of the structural features.

[1] Huang Z.L., Drillon M., Masciocchi N., Sironi A., Zhao J.-T., Rabu P., Panissod P., *Chem. Mater.*, 2000, **12**, 2805. [2] Abdelouhab S., François M., Elkaim E., Rabu P., *Solid State Sciences*, in press.

Keywords: lamellar hybrid compound, transition metal, structure-properties relationship

P.08.14.9

Acta Cryst. (2005). A61, C342-C343

Structures of New Molecular Conductors Based on Functionalized Organic Donors

Leokadia Zorina^a, Rimma Shibaeva^a, Salavat Khasanov^a, Sergey Simonov^a, Lyudmila Kushch^b, Eduard Yagubskii^b, Cecile Meziere^c, Stephane Baudron^c, Patrick Batail^c, Enric Canadell^d, ^aInstitute of Solid State Physics, RAS, Chernogolovka, Russia. ^bInstitute of Problems of Chemical Physics, RAS, Chernogolovka, Russia. ^cChimie Inorganique, Matériaux et Interfaces, CNRS-Université d'Angers, France. ^dInstitut de Ciencia de Materials de Barcelona (CSIC), Bellaterra, Spain. E-mail: zorina@issp.ac.ru

Functionalized organic donors are remarkable for the ability to form hydrogen bonds of cation...cation and cation...anion types, which can effectively control the crystal architecture of molecular conductors [1]. Hydrogen bond network is well developed in the crystals of four new radical cation salts based on amide functionalized EDT-TTF donors EDT-TTF-CONH₂ (D1) and EDT-TTF-(CONH₂)₂ (D2) [2].

Semiconducting α' -(D1)₄[FeNO(CN)₅] (1), α' -(D1)₄[Co(CN)₆] (2), β -(D1)₆[Fe(CN)₆] (3) and (D2)₄[FeNO(CN)₅]NB (4) salts have been prepared and characterized by X-ray single crystal diffraction experiments and band structure calculations. (D1)₂-dimers or (D2)_n-extended zigzag chains of donors connected through functional groups are found to be stable structural motifs in 1-4. The 1 and 2 salts are isostructural but contain anions of different charge, -2 and -3, respectively. The degree of charge transfer affects on electronic structures of the crystals that results in changing their transport properties: $\sigma_{RT}(2)/\sigma_{RT}(1)=50$. In the crystals 4 a superstructure with