molecules assumed as a protection again spontaneous crystallization in organisms? **Acknowledgements:** The support by the Grant Agency of AS CR under grant no. IAA100100915 is gratefully acknowledged.

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Keywords: molecular packing, space-group frequencies, crystallization

MS17.P21

Stacking interactions between phenanthroline ligands in square-planar complexes

Dragan B. Ninković,[a,d] Goran V. Janjić,[c] Predrag V. Petrović,[a] Snežana D. Zarić,[b]   [a]*Innovation center of the Department of Chemistry, Studentski trg 12-16, 11000 Belgrade, (Serbia).* [b]*Department of Chemistry, University of Belgrade, Studentski trg 12-16,11000 Belgrade, (Serbia).* [c]*IHTM, Njegoševa 12, 11000 Belgrade, (Serbia).* [d] E-mail: dragannin@yahoo.com

Noncovalent interactions of π-systems, including stacking interactions, have been extensively studied in recent years. Stacking interactions are generally studied between aromatic organic molecules or fragments. However, it was shown that other planar molecules and fragments can be also involved in stacking interactions.

Stacking interactions between chelate and C_6-aromatic rings were recognized by analyzing the data in crystal structures of square-planar transition metal complexes from the CSD. In the crystal structures there are mutual slipped-parallel orientation of these rings, similar to the orientation of two benzene rings. Recently we showed the existence of chelate-chelate stacking interactions in crystal structures from CSD [1]. Geometrical analysis of stacking interactions with aromatic nitrogen-containing ligands show that nitrogen-containing aromatic rings usually form slipped parallel alignment where most of the ring-plane area overlaps [2].

Phenanthroline (1,10-phenanthroline-N,N') (phen) molecule coordinating to a metal ion forms large planar system of four rings: two pyridine fragments, one C_6-ring and one chelate rings. This planar system has propensity to form stacking interactions with the π -system of various aromatic groups. Tendency for stacking interactions is important for using these complexes in biochemistry, supramolecular and medicinal chemistry.

To understand better stacking interactions of phen complexes, here we analyze the geometry of stacking interactions between phen square planar metal complexes in crystal structures from the CSD.

In the Cambridge Structural Database (CSD) 61 structures with 172 stacking interactions of phen square-planar complexes were found [3]. The results of crystallographic analysis show that in most of the structures two interacting ligands are oriented "head-to-tail", with the large area of phen ligand involved in the overlap. Phen complexes show large range of different overlap geometries in stacking interactions, however, short metal-metal distances were not observed. Stacking interactions of phen square-planar complexes form chains and dimers in crystal structures.

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Keywords: Stacking interaction, Intermolecular interaction, Crystal structures

MS18.P01

Structure and magnetic properties of nanoparticles $Ni_{0.5}Zn_{0.5}Cr_{0.1}Fe_{1.9}O_4$

L. M. Salah, E. Ateia, A. A. H. El-Bassuny, *Physics Department, Faculty of Science, Cairo University, Giza, (Egypt).* E-mail: lobnasalah2003@ yahoo.com

Nanostructure ferrite of composition $Ni_{0.5}Zn_{0.5}Cr_{0.1}Fe_{1.9}O_4$ was prepared by sol–gel, co-precipitation, citrate-gel, flash and oxalate precursor methods. Structural and micro structural analysis of all the samples were carried out (XRD, IR, TEM, SEM and AFM) . The saturation magnetization at room temperature was also studied. Lattice constant and particle size were determined by different methods. The average values of the crystal size for different method were in nanometric range (5 - 75 nm). It was observed that the lattice parameter of cubic spinel was not varied and the positions of the tetrahedral and the octahedral band are not shifted which give the indication that the cation distribution are the same. So, the results of magnetic hystersis were explained in terms of the relation between grain size and magnetic properties in addition to surface randomizing effect in nanocrystals leading to superparamagnetism state.

Keywords: nanocrystals, synthesis, ferrite.

MS18.P02

Identification of single photoswitchable molecules in nanopores of silica xerogels using neutron powder diffraction

Dominik Schaniel,[a] Theo Woike,[b] A. Cervellino,[c] Lukas Keller,[d] Jürg Schefer,[d]   [a]*Laboratoire de Cristallographie, Résonance Magnétique et Modélisation (CRM2), Institut Jean Barriol, Nancy Université, Nancy (France).* [b]*Institut fuer Strukturphysik, TU Dresden, Dresden (Germany).* [c]*Swiss Light Source (SLS), Paul Scherrer Institute, Villigen PSI (Switzerland).* [d]*Laboratory for Neutron Scattering (LNS), Paul Scherrer Institute, Villigen PSI (Switzerland).* E-mail: dominik. schaniel@crm2.uhp-nancy.fr

Single photo-switchable molecules of $(CN_3H_6)_2[Fe(CN)_5NO]$ (GuNP) are embedded into nanopores of a SiO_2 xerogel. We show that it is possible to identify the structural motif (fingerprint) of the embedded complex by analyzing neutron powder diffraction data in a limited Q range (Q<37 nm^{-1}) using the Debye approach. The structural study reveals that the pores are occupied by GuNP-monomers with a fill factor of 60-80%. The mutual arrangement of the anion and cation in the GuNP monomer is slightly changed (~ 1% elongation) while the bond lengths within anion and cation are changed by less than 0.2% with respect to the single crystalline form of GuNP.

This example demonstrates that the structure of single molecules in nanopores and their distance to nearest neighbors of the host network can be analyzed using a standard neutron powder diffractometer with limited Q-range such as DMC@SINQ. From the analysis of the small angle range one obtains an estimate for the average pore size and the fill factor of pores with embedded complexes. The distance between atoms of the host network and the guest complexes can be determined from the intermediate scattering range. Assuming a sufficient scattering contrast between host and guest this method can be extended also to the x-ray case, such that these experiments can be performed on laboratory

P.MS.18

x-ray sources. Hence we have shown that such nanostructured materials can be characterized using standard powder diffraction sources. Results are published in [1].

[1] A. Cervellino, J. Schefer, L. Keller, Th. Woike, D. Schaniel, *J. Appl. Cryst.* **2010**, *43*, 1040-1045.

Keywords: debye approach, nanomaterial, powder diffraction

MS18.P03

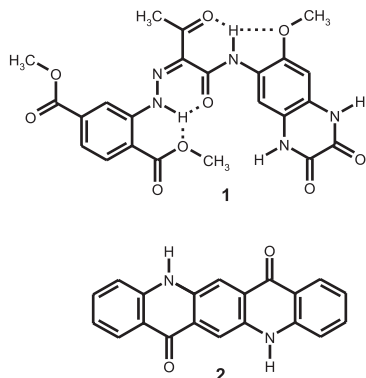**Pair-distribution function analyses of nanocrystalline organic pigments**

Martin Schmidt,ᵃ Lothar Fink,ᵃ Edith Alig,ᵃ Christian W. Lehmann,ᵇ Claudia Weidenthaler,ᵇ *ᵃInstitut für Anorganische und Analytische Chemie, Goethe-Universität, Frankfurt am Main (Germany). ᵇMax-Planck-Institut für Kohlenforschung, Mülheim (Germany).* E-mail: m.schmidt@chemie.uni-frankfurt.de

The pair-distribution function (PDF), represents the probability to find two atoms with an interatomic distance r. The PDF is generally used to investigate local structures of disordered, nanocrystalline or amorphic inorganic compounds, liquids and glasses. Here, the PDF analysis is applied to nanocrystalline organic pigments, having domain sizes of 3 - 30 nm.

Pigment Yellow 213 (**1**) exists in two crystal phases. The structure of the yellow α-phase was solved from X-ray powder data with the help of electron diffraction. The brown β-phase shows only a few broad humps in the X-ray powder diagram. Its PDF analysis, based on synchrotron data, reveals, that the molecules are arranged in stacks. From the PDF curve, the domain size is determined to be about 3 nm in stack direction, and the local structure is found to be similar to the α-phase. [1]

The α^{II}-phase of quinacridone (Pigment Violet 19), **2**, is nanocrystalline, too. [2] Powder patterns of all four phases of **2** were recorded on laboratory STOE Stadi-P diffractometers in transmission mode, using Cu-$K\alpha_1$ and Mo-$K\alpha_1$ radiation, at temperatures from 100 K to 400 K. The PDF analyses proved that the local structures of the α^I, β and γ-phases are considerably different; in contrast the local structure of the α^I and α^{II}-phases have similarities, although their X-ray powder patterns are different.

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Keywords: pair-distribution function analysis, pigment, local structure

MS18.P04

X-ray powder diffraction study of particle sizes of metastable Ru_xM_{1-x} (M = Ni, Cu)

Alexey Alexeyev, Alexander Borodin, *Nikolaev Institute of Inorganic Chemistry Siberian Branch of the Russian Academy of Sciences (Russia).* E-mail: alexeyev@niic.nsc.ru

Transition metal alloys with ruthenium are efficient catalysts in Fischer-Tropsch synthesis. One way of preparing bimetal alloys as nanoparticles is thermal decomposition of appropriate binuclear complexes at 200-600°C. In this work, we studied thermal decomposition products of $[M(PyO_2)_2RuNO(NO_2)_4OH]$ M = Ni, Cu complexes at 300, 350, and 400°C.

Initial binuclear complexes were prepared by mixing equimolar amounts of $M(NO_3)_2$ M = Ni, Cu and $Na_2[RuNO(NO_2)_4OH]$ with pyridine-N-oxide (3 equivalents) in acetone.

In the both cases, thermal decomposition was performed on a TG 209 F1 Iris micro thermobalance (NETZSCH) in hydrogen atmosphere. Annealing was executed for 6 h at each temperature point with heating rate of 1 degree/min. The mass loss fits the calculated that within ± 2%.

X-ray diffraction study of thermolysis products was carried out on a Shimadzu XRD7000 diffractometer (CuKα-radiation, Ni-filter) at the ambient temperature. Upon decomposition of $[Cu(PyO_2)_2RuNO(NO_2)_4OH]$, two-phase material containing solid solutions based on the copper HCC and the ruthenium HCP cells was revealed to form. The particle sizes calculated by the Scherrer formula are ~ 4 nm for T = 300 and 350°C and 7 nm for 400°C. With decomposition of $[Ni(PyO_2)_2RuNO(NO_2)_4OH]$ at all temperatures mentioned, one-phase products formed, namely, solid solutions with the particle sizes of 4 nm and based on ruthenium HCP cell, Ru_xNi_{1-x} x = 0.68-0.75. The composition was estimated by the Retgers rule. Most likely a portion of nickel is amorphous, as further annealing of one sample at 850°C for 10 h resulted in two crystalline phases on the basis of ruthenium (60 % in mass) and nickel (40 % in mass). The compositions of the phases are near the corresponding boundaries of the two-phase range of the phase diagram.

Keywords: x-ray, ruthenium, nano

MS18.P05

Synthesis, structure and properties of nanosized titanium dioxide with η-TiO$_2$ modification

Galina M. Kuzmicheva,ᵃ Lubov' N. Obolenskaya,ᵃ Elena V. Savinkina,ᵃ Nina A. Prokudina,ᵃ Alexey A. Natykan,ᵇ Denis N. Titov,ᵃ Vladimir V. Chernyshov, ᵇ *ᵃDepartment of Solid State Physics and Chemistry, Lomonosov State Academy of Fine Chemical Technology, Moscow. ᵇInorganic Chemistry Department, Moscow State University, Moscow.* E-mail: galkuz@orc.ru

In recent years, great attention has been focused on TiO$_2$ materials because they exhibit a variety of controllable electronic and optical properties and have extensive applications. TiO$_2$ is proved to be a good and perspective active component for different types of catalysts and photocatalysts. In comparison with other semiconductor catalysts, TiO$_2$ is biologically and chemically inert, stable to photodegradation, and also relatively cheap.

There are 12 polymorphic TiO$_2$ modifications in both bulk and nanoscale forms, but the η-TiO$_2$ phase was obtained only in the nanostate and rather scarcely characterized. One of the promising methods of its synthesis, a sulfate method, allows preparing nanosized