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

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

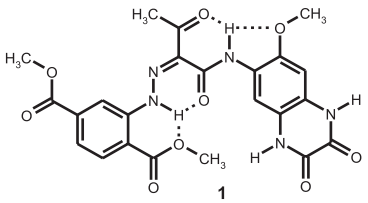
Martin Schmidt,[a] Lothar Fink,[a] Edith Alig,[a] Christian W. Lehmann,[b] Claudia Weidenthaler,[b] [a]*Institut für Anorganische und Analytische Chemie, Goethe-Universität, Frankfurt am Main (Germany).* [b]*Max-Planck-Institut für Kohlenforschung, Mülheim (Germany).* E-mail: m.schmidt@chemie.uni-frankfurt.de

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 $\alpha^{II}$-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 $\alpha^{I}$, β and γ-phases are considerably different; in contrast the local structure of the $\alpha^{I}$ and $\alpha^{II}$-phases have similarities, although their X-ray powder patterns are different.

[1] M.U. Schmidt, S. Brühne, A.K. Wolf, A. Rech, J. Brüning, E. Alig, L. Fink, C. Buchsbaum, J. Glinnemann, J. van de Streek, F. Gozzo, M. Brunelli, F. Stowasser, T. Gorelik, E. Mugnaioli, U. Kolb, *Acta Cryst* **2009**, *B 65*, 189-199. [2] E.F. Paulus, F.J.J. Leusen, M.U. Schmidt, *CrystEngComm* **2007**, *9*, 131-143.



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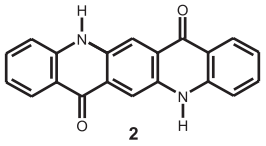

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**Keywords: pair-distribution function analysis, pigment, local structure**

## MS18.P04

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**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

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**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] [a]*Department of Solid State Physics and Chemistry, Lomonosov State Academy of Fine Chemical Technology, Moscow.* [b]*Inorganic 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