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XRPD structural studies of new group of coordination polymers

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In our study we have synthesized a group of new coordination polymers with general formula CdX_2R_2, where X is Br, Cl or I, and R is aliphatic or aromatic amine. According to the kind of central atom and inorganic anion X used, there is a possibility of obtaining structures with different spatial arrangement. Obtained compounds form various structures, from isolated molecules similar to cis-platinum, isolated polymeric chains, polymeric chains crosslinked into layers to three dimensional systems.

Powder diffraction experiments were carried out using synchrotron radiation on synchrotron PETRA III. The usage of synchrotron radiation has led to a proper solution of investigated structures from powder data. Crystal structures were solved using EXPO [1] program, Rietveld refinement was performed using Jana2006 [2].

Presented group of coordination polymers consist of six compounds, all crystallize in monoclinic crystal system. Compounds of $CdCl_2$ and $CdBr_2$ with linear amines form systems of cadmium-halide chains bridged by diamines. $CdCl_2(NH_2C_6H_4NH_2)_2$ creates a three dimensional structure in which aromatic amines connect inorganic chains. In the case of $CdI_2(NH_2C_6H_4NH_2)_2$ isolated chains are formed, in which each aromatic amine bridges two cadmium atoms.

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Application of synchrotron data to PDF-based structure refinement

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Atomic pair distribution function (PDF)[1] is a direct space-based relation between interatomic distances and the number and scattering power of atoms corresponding to said distance. PDF is directly obtainable from properly normalized and corrected powder diffraction data registered in a wide Q range ($Q=4\pi/\lambda\sin\theta$). Necessity for a wide Q range arises from the truncation errors in the Fourier series summation observable as ripples in resulting function. In inlab experiments, Mo or Ag sources have to be employed to allow for a sufficient data range. Another choice is synchrotron radiation with its superior intensity and selectable measurement wavelength.

PDF contains diffuse scattering information (if present) and may be used in studying structures with local ordering. Also, nanocrystalline samples as well as amorphous phases are studied with PDFs.

Results of crystal structure refinements using PDFGUI[2] based on the PDFs obtained with PDFGETX3[3] from synchrotron data are presented.

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