Focus on the lightest atoms in the smallest crystals

Scientists from the Institute of Physics of the CAS lead an international team, which developed a new method to analyze the scattering of electrons in nanocrystals. The method is so accurate that it can be used to detect the positions of even the lightest of all atoms – the hydrogens. The accuracy and reliability of the method was demonstrated in a publication, where hydrogen positions were determined in two different materials. The work was published in the journal Science in its January 13th, 2017 issue.

Structural crystallography is a scientific discipline focused on the determination of atomic structure of crystalline materials. The knowledge of crystal structure is crucial for many research fields like material science, organic and inorganic chemistry, pharmacology and molecular biology. Despite the dramatic progress structural crystallography has made over the last century, problems remain that are impossible or very hard to tackle. One of them is a reliable structure analysis of nano- and microcrystals, i.e. crystals with dimensions around one micrometer or smaller. This represents a severe problem in many fields, where the materials of interest do not form sufficiently large crystals, like synthetic chemistry of new materials, discovery of new catalysts for chemical industry, development of new drugs or geosciences.

Important progress has been made also in the field of analysis of nanocrystals, thanks to the development of new techniques exploiting scattering (diffraction) of electrons on crystals. So far, however, this method provided only approximate information and did not allow the determination of all necessary details of the crystal structures. An international team led by the scientists from Department of Structure Analysis of the Institute of Physics of CAS has therefore spent last few years developing a method, which would lift this limitation and improve the accuracy of structure analysis by electron diffraction. The goal has been achieved by using advanced computing techniques and development of new algorithms for data processing.

The success of the new method is demonstrated by determination of the positions of the lightest of all atoms – atoms of hydrogen. A hydrogen atom contains only one proton and one electron, and its signal in electron diffraction is the weakest signal among all chemical elements. A reliable detection of hydrogen atom positions is generally considered as one of the most difficult tasks in structure determination, and it was so far essentially impossible with electron diffraction. The work was conducted in collaboration with scientists from CNRS Caen, France, and it was published in the prestigious journal Science. Within the work, two structures were analyzed – an organic compound paracetamol, which is the active ingredient of several pain killing and fever reducing drugs, and hydrated cobalt aluminophosphate (CAP). The latter was selected as a representative of the class of framework materials, which are commonly used in chemical industry as sorbents and catalysts. In both cases all hydrogen positions in the crystal structure were found.

The method brings a qualitative progress in the capacity of analysis of crystal structures. Given the wide applications of crystallography in natural science, the method has the potential to contribute to the development of many scientific fields.

Reference:

Hydrogen positions in single nanocrystals revealed by electron diffraction. L. Palatinus, P. Brázda, P. Boullay, O. Perez, M. Klementová, S. Petit, V. Eigner, M. Zaarour and S. Mintova, *Science* (2017).

http://science.sciencemag.org/

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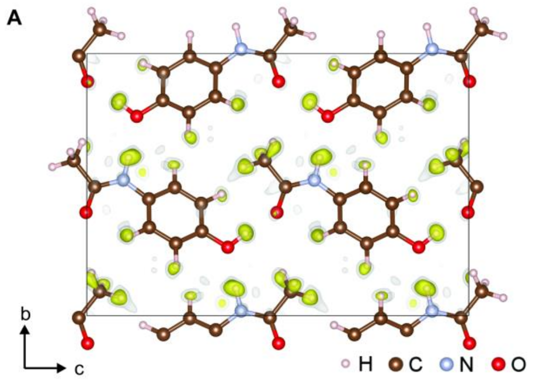
Figure captions:



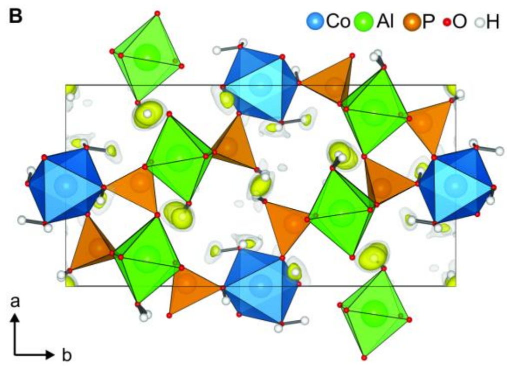


Figure "TZ_Science_vodiky_A.png" & figure "”TZ_Science_vodiky_B.png": Structure of (A) paracetamol form II and (B) cobalt aluminophosphate with superimposed difference electrostatic potential (gray and yellow isosurfaces). The maxima of the potential correspond to the positions of hydrogen atoms.

The video of the structure of paracetamol is also available: http://www-xray.fzu.cz/press/hydrogens_in_paracetamol.mp4

The video of the structure of cobalt aluminophosphate is also available: http://www-xray.fzu.cz/press/hydrogens_in_CAP.mp4

Figure "Cover_Science_vodiky.jpg": The topic of the paper of L. Palatinus et al. was featured also on the cover of the Science journal, issued on January 13th, 2017.