s2.m10.p3 **Charge density study of "blue protein model compounds".** Marek Fronc,[a] Jozef Kozisek,[a] Hartmut Fuess[b] and Carsten Paulmann[c], [a]*Department of Physical Chemistry, Faculty of Chemical and Food Technology, Slovak University of Technology, SK-81237 Bratislava, Slovakia,* [b]*Materials Science, Darmstadt University of technology, D-64287 Darmstadt, Germany, and* [c]*Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee, D-20146 Hamburg, Germany. E-mail: fronc@chelin.chtf.stuba.sk*

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The importance, which the blue proteins play in the electron-transfer processes in the living organisms, makes them very interesting subjects of scientific research. Unfortunately, natural blue proteins are usually too large to be studied by more sophisticated methods. Instead so-called model compounds, which have the similar properties as the active center of the protein are used. We are studying the distribution of the electron density in the compounds of Cu(I) and Cu(II); [Cu(bite)](BF_4) which corresponds to the reduced form and [Cu(bite)]$(BF_4)_2$ which represents oxidized form of the redox couple (bite = biphenyldiimine dithioether, $C_{28}H_{22}N_2S_2$) [1]. Data were collected by use of synchrotron radiation source (λ = 0.5604 Å) at synchrotron beamline F1 at HASYLAB/DESY, Hamburg at 100 K. For corrections, integration and data reduction programs SAPRO, SAINT, ABSORB and SORTAV were used. Multipole refinement was performed with XD software package. For the [Cu(bite)](BF_4) charge density maps show non-bonding interaction between Cu and N at distance 1.929 (2) Å and between Cu and S at distance 2.3148(5) Å. Lone pair of the S at shorter distance 2.17 86(5) Å points towards the electron deficiency space of the Cu, as well as the lone pair of the nitrogen at distance 1.960(2) Å. Charge density studies on [Cu(bite)]$(BF_4)_2$ are currently in progress [2].

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s2.m10.p4 **Site-dependent atomic response on an external electric field in $GaPO_4$: New insights into understanding the inverse piezoelectric effect.** S.V. Gorfman[1,2], V.G. Tsirelson[2], U. Pietsch[1], [1]*Institute of Physics, Potsdam University, Am Neues Palais 2, 14469, Potsdam, Germany,* [2]*Quantum Chemistry Department, Mendeleev University of Chemical Technology, 121047, Moscow, Russia. E-mail: sgorfman@rz.uni-potsdam.de*

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This work elucidates the microscopic origin of the inverse piezoelectric effect in $GaPO_4$ using X-ray diffraction technique. Our approach is based on recently developed theory of X-ray diffraction by a crystal in an external electric field [1]. It was shown that the electric-field induced change in the X-ray diffraction intensities can be expressed via the displacements of pseudo-atomic fragments from their equilibrium positions. We derived an explicit expression for these displacements, taking into account the phonon properties of a crystal lattice, and worked out a corresponding model of X-ray structure factors. The relative changes in experimental intensities induced by external electric field in $GaPO_4$, were collected at the D3 beamline at HASYLAB (Hamburg). Preliminary calculations based on the simplified models describing atomic displacements were used to select those reflections and the wavelengths, at which reflections are most sensitive to the microscopic changes caused by the electric field. Due to experimental problems, the measured X-ray intensity set consists of 18 reflections: that is not enough to find a unique solution in terms of the general model of electric-field induced atomic displacements. Therefore, the number of model parameters describing the atomic displacements was reduced by introducing some additional constraints (apart from symmetry ones). We applied the constraint, which follows from previous density functional calculations [3], in which was found that SiO_4 tetrahedra in quartz rotate as nearly rigid units. Therefore, considering $GaPO_4$ with the same structure we have fitted our model to the experimental X-ray intensities keeping the bond lengths nearly fixed. The rotations of GaO_4- and PO_4-tetrahedra in the external electric field were considered independently. In the framework of this approach, the atomic origin of the inverse piezoelectric effect can be described by the electric-field induced rotation of slightly distorted MO_4 tetrahedra and the subsequent polarization of the charge density within a unit cell. We have also tested other structural models and found that they failed to fit the experimental data properly if the rotational character of the atomic displacements is ignored.

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