all play. Although we are all using the same ball, confusion reigns because we each play the game according to our own set of rules. A good chemical model requires well defined concepts that lead to quantitative predictions. The ionic model meets these criteria. The electroneutrality rule (the sum of all atomic valences in a compound is zero) is the only assumption the model makes and it applies to all compounds that obey this rule (mostly inorganic compounds, but also aqueous chemistry, hence much of biological chemistry). From the Coulomb field of the ionic model one can derive rigorous concepts of atom, bond, atomic valence, bond valence and electronegativity as well as Lewis acid and base strength. The result is a predictive model expressed in terms of the familiar chemical concept of localized bonds linking nearest-neighbour atoms.

Keywords: bonding, ionic model, bond valence model

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Structure of KTP crystals grown by top-seeded solution and spontaneous flux crystallization methods

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Crystals of the potassium titanyl phosphate $KTiOPO_4$ (KTP) family are under investigation for number years because of their application in nonlinear optics. X-Ray study of KTP single crystals grown by the top-seeded solution and spontaneous flux crystallization methods was made to evaluate the influence of growth conditions on the crystal structure and to use these results for further investigations of the structure of KTP crystals doped by isovalent and heterovalent impurities. X-Ray measurements were performed at room temperature using the four-circle CAD-4F Enraf Nonius diffractometer for the half of the sphere of reciprocal space up to $(\sin\theta/\lambda)_{max}=1.22$. Both structures were refined using the JANA2000 program up to $R=0.013$, $R_w=0.021$ for the case of the top-seeded solution method and up to $R=0.017$, $R_w=0.025$ for the case of the spontaneous flux crystallization. It was established that the electron structure of KTP crystals grown by these two methods was related with the defect structure of these crystals. The greater number of defects is shown to be formed in crystals grown by the spontaneous flux crystallization method. At the same time the similarity of potassium sublattice disordering, of cell parameters and of middle interatomic distances in structures is observed. The work was done with the partial support of the Grant for the leading scientific schools NSh-2192.2008.5 and the "Russian Science Support Foundation".

Keywords: structure and charge-density analysis, structure-properties relationships, nonlinear optical materials

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Anomalous SAXS for the morphology and metal content of a metallothionein in a metal-atom replacement

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Metallothioneins (MTs) are cysteine-rich proteins that have a high affinity with heavy metal ions. In this study, a protein unfolding-refolding process is developed to replace the metal atoms of cadmium-zinc MTs by Cu(I) or Cu(II). Using small angle X-ray scattering (SAXS) and anomalous SAXS, we have studied the changes of morphology and metal content of the MT in the designated metal-atom replacement process. The SAXS results reveal that the Cd-Zn MT has a rod-like shape and a radius of gyration $Rg = 26$ Å; in the solution of 4 M urea and 0.1 M ß-ME, the protein is unfolded and the metal atoms are stripped from the protein, leading to a smaller Rg of 22 Å. With the unfolding environment replaced by a solution rich in Cu(I), the modified MT cannot correctly refold, but forms oligmers of a rod-like shape with a much larger Rg value of 42 Å; when the refolding process proceeds with Cu(II), the modified MT can closely refold to the native morphology of the wild-type Cd-Zn MT. Anomalous SAXS, with the X-ray energy tuned close to the K-edge absorption of Cu, clearly indicates that the refolded MT contains Cu atoms after the refolding process. From the decrease of the ASAXS intensity, we have estimated the copper content in the modified Cu-MT. Dummy residue simulation is used to approximate the unfolded and refolded protein morphologies from the SAXS data. The Cu-S bonding observed in the X-ray absorption at the Cu K-edge and UV-VIS absorption spectra indicates clearly that Cu atoms occupy the original metal sites of the MT after the metal-atom replacement process. Corresponding changes in the circular dichroism of the MT due to the metal-atom replacement are also observed. The different influences of Cu(I) and Cu(II) in the refolding of the MT are discussed.

Keywords: anomalous SAXS, metallothionein, metal atom replacement

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Synchrotron SAXS reveals structural organization of iron oxide nanoparticles in aqueous solutions

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Iron oxide particles prepared in docosane (DOC7-PEG-PL) and octadecane OC11-PEG-PL [1] and covered with PEGylated phospholipids to make them water soluble were analyzed by small-angle X-ray scattering (SAXS). The low-resolution structures of the iron oxide cores were reconstructed *ab initio* using DAMMIN [2]. Typical shapes of the DOC7-PEG-PL (a) and OC11-PEG-PL (b) cores (inserts in Figure) yield good fits to the experimental data (curves 3). The density of the iron core of the DOC7-PEG-PL nanoparticles decreases from the center to periphery, whereas the OC11-PEG-PL sample displays a double layered structure. These differences are related to the dissimilarity of the magnetic properties of the specimens. The nanoparticles were found to form clusters containing 3-4 densely packed cores due to magnetic interactions, and their spatial organization was analyzed by the program SASREF

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