structure (interatomic distances and atomic displacements) from regular positions structure was perfomed. In particular, the insignificant shifts of cations and the essential shifts of anions from the initial ideal positions of the supercell were established [2], [3].

[1] Gale J., *GULP user manual*, Royal institution and Imperial College, London, 1992. [2] Urusov V.S., Petrova T.G., Eremin N.N., *D. Akad. Nauk*, 2002, **47**, 811. [3] Urusov V.S., Petrova T.G., Eremin N.N., *D. Akad. Nauk*, 2003, **392**, 469.

Keywords: solid solution, computer modeling, mixing properties

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The Vibrational Properties of Katoite $Ca_3Al_2[(OH)_4]_3$: A Periodic *Ab-initio* Study

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The vibrational spectrum of katoite was simulated by using the periodic *ab initio* CRYSTAL program [1].

In spite of the structural similarities with garnets [2], katoite presents a quite different spectrum, due to the presence of hydrogen atoms and lack of connectivity among the $Al(OH)_6$ octahedra. A deep analysis of the dynamical-matrix eigenvectors, including isotopic substitutions and modes visualization, was performed in order to assign the 345 modes. Hydrogen related modes, namely OH strectching, AlOH bending and H rotation with respect to the Al-O axis can be identified as nearly pure modes, although only the former form a separated band.

For the OH strectching, anharmonicity effects, that are as large as 150 cm^{-1}, have been taken into account. The calculated values are in very good agreement with available experimental data. [3]

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Keywords: ab-initio calculations, hydrogernet, vibration

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3D Model of Ternary Complex of Human 3β-HSD type I. Rational Mutagenesis

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Mammalian 3β-Hydroxysteroid Dehydrogenase/Isomerase (3β-HSD) catalyzes conversion of dehydroepiandrosterone and pregnenolone to active hormones, progesterone and androstenedione. A 3D model of ternary complex of human 3β-HSD type I complexed with NAD cofactor and androstenedione product has been developed based upon two X-ray structures, the UDP-galactose 4-epimerase (UDPGE) complexed with an NAD cofactor and substrate, and the 17β-hydroxysteroid dehydrogenase (17β-HSD) complexed with an NADP cofactor and the androstenedione substrate. These enzymes share 21% and 15% sequence identity with 3β-HSD_1 enzyme in the overlapping regions. The cofactor and substrate binding sites in 3β-HSD_1 resemble the corresponding sites in UDPGE and 17β-HSD structures. A dimer structure of 3β-HSD_1 with a stereochemically optimal interface was built by respective 3D superposition with both subunits of dimeric structure of DTDP-D-glucose 4,6-dehydratase with which 3β-HSD shares 19% sequence identity. The 3D structure of 3β-HSD enzyme is in good agreement with existing biochemical data and is being used to design rational mutations to elucidate key substrate binding residues in the active site and the basis for enzyme dual oxidoreductase and isomerase functions. As predicted by the 3D model, mutagenic data have confirmed a role for H232 in recognizing the 17-keto group of the bound substrate. The H232A mutant lacks the oxidoreductase activity but retains the isomerase activity.

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Keywords: 3D model, structure/function relation, mutagenesis

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Force Field Parameters for the Photosystem II Reaction Center

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Our recent experimental results [1] led to the hypothesis that at a room temperature the reduced pigment pheophytin *a* (PHO) induces conformational changes of the photosystem II reaction center (PSII RC) pigment-protein complex. The conformational changes affect excitonic interaction of the RC chlorophylls, which was observed in absorption and CD spectra. In order to better interpret our experiments, theoretical approach such as molecular dynamics simulation is useful tool through the use of dynamic conformational analysis of PSII RC. At present the complete force field (FF) parameters applied in MD are not available for the photosynthetic pigments of PSII RC, namely partial atomic charges and force constants of chlorophyll *a*, plastoquinone and both neutral and reduced form of PHO. From that reason we have developed new FF parameters calculated by quantum chemical method on the pigments with known experimental 3D structure. New FF parameters were successfully applied in preliminary MD simulations on the pigment-protein complex PSII RC (experimental structure pdbID 1S5L). This work is supported by MSMT (MSM6007665808, GACR206/02/D177) and by AVCR (AVOZ60870520).

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MAIN 2004: Model Building beyond 100 Residues per Minute

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Model building of macromolecular structures at moderate resolution (around 2.8A and below) still requires user intervention to resolve the potential chain trace ambiguities, however, the classical approach by which amino acids are edited manually on one by one basis is becoming history. After an electron density map has been converted to a skeleton, the skeleton is used for recognition of secondary structure and main chain trace directly. Two consecutive screw turns are recognized as a helical structure, whereas beta structures are recognized from straight stretches of skeleton corresponding to at least five amino acids and their arrangements in pairs or sheets. After the secondary structure elements are established a combinatorial search of possible connectivities is used to further reduce the main chain ambiguities. The remaining ambiguities can be further resolved interactively by manual editing of the skeleton. The resolved skeleton then serves for building of the first main chain trace based on sp3 fragments positioned at the potential CA positions. If the resulting model looks satisfactory, it is converted to amino acid residues and enters refinement. Otherwise the resulting models can at any stage continue along the classical path of automated and manual model rebuilding, still using the same program with the same interactive 3D graphical user interface. (See http://www-bmb.ijs.si/)

Keywords: computational methods, crystallographic software, macromolecular crystallography