biological diffractometer (IBARAKI Biological Crystal Diffractometer: iBIX) at BL03, in Material and Life Science Facility in J-PARC. The diffractometer is designed to cover samples that have their cell edges up to around 135Å with a resolution up to 1.2Å (biological macromolecules) and to 0.7Å (organic compounds). In 2008, the basic part of the instrument of iBIX, including 14 detectors (a two dimensional detector which consists of ZnS:Ag/$^{10}B_2O_3$ scintillators with a wavelength shift fiber system, and the total solid angle of the detector system: 9%) has been completed to prepare for diffraction experiment. Since the end of December in 2008, iBIX bas been opened for users. Neutron diffraction datasets of several organic compounds of the known structure have been collected by using the iBIX and molecular structures obtained from the analysis agreed with the reported structures.

We have tried to collect the first TOF neutron diffraction dataset of a protein crystal by using iBIX in order to estimate the performance and characteristics of iBIX. The selected crystal for the purpose is ribonuclease A(RNase A) soaked in heavy water. The crystal volume was 4.7 mm^3. The cell parameters were a=30.4Å, b=38.6Å, c=53.4Å, b=105.8º in a monoclinic form, respectively. Measurement conditions are as follow: the accelerator beam power: 120kW, the pulse repetition: 25Hz, the range of wavelengths: 1.5~4.5Å (the 1st frame), 4.2~7.5Å (the 2nd frame), the number of measurement settings: 100 settings (1st frame: 67settings, 2nd frame: 43 settings), the exposure time: 5 hours/setting (the 1st frame), 1 hour/setting (the 2nd frame), the total amount of measurement time for full dataset: 17 days.

The data reduction (to extract a HKLF list from raw data) was carried out by using a new data processing software "STARGazer" which we have developed for TOF neutron diffraction data. The data reduction for almost all of the both frame data was finished and consequently HKLF list was obtained. The completeness of Bragg reflections is 88.8% of 1.7Å resolution. The structure refinement was carried out with this intensity dataset. We have succeeded in obtaining the reasonable structure after the structure refinement by comparing with the already-reported structure [1]. After accelerator power will become 1MW in J-PARC and the total number of detector for iBIX will become 30, the full dataset of standard sample RNase A which is 1mm^3 in volume can be collected in about 3 days.

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Keywords: TOF neutron diffractometer, protein crystallograpy, RNase A

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Crystallographic autostereograms

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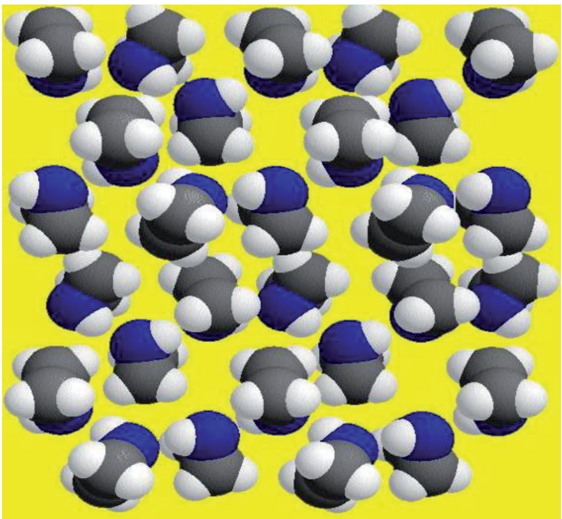
Crystallographic studies are inherently connected with the drawings of crystal structures on publications pages or on computer screens. Various methods have been worked out for facilitating the 3-dimensional arrangements of atoms in 2-dimensional drawings. The most commonly used were stereoscopic pairs, which were prepared after computers could be used for drawing crystal structures [1]. The in-depth viewing of stereopairs required stereoscopes, although it was pointed out (cit.) "that most readers – maybe after a little practice – should be able to achieve stereopsis without mechanical aid" [2]. Recently stereopairs are seldom found in scientific publications, owing to commonly used computers allowing crystal structures to be easily processed and viewed in any style and at any chosen direction. This possibility somewhat degraded the value of clear presentations of crystal structures in crystallographic publications.

Alternative methods for perceiving 3-dimensional crystal structures were also presented. One is based on the concept of autostereograms, or single-image stereograms [3]. Autostereograms can be used not only for scientific publications, but also for artistic presentations of crystal structures.



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Keywords: stereographic, crystal structure, illustration

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Incorporation of crystallographic data use into undergraduate chemistry education

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Nearly every chemistry course in an undergraduate chemistry major's curriculum contains a significant number of topics that can be illustrated or enhanced through use of crystallographic information. This presentation will describe specific examples of the use of crystallographic information in a wide range of chemistry courses. At the General Chemistry level, students learn the basic VSEPR geometries and are faced with need to visualize molecules in three-dimensions. Manipulation, *in silico*, of examples whose coordinates are derived from crystal structures is perhaps the most obvious use. Students are also faced with consideration of evaluating the relationships between bond lengths and bond enthalpies and direct investigation of actual molecular structures is of value. In Organic Chemistry, students can examine specific molecular structures to better understand the 3-D nature of molecules. (Unlike a typical drawing on paper, benzophenone is not flat.) In Physical and Analytical Chemistry, the potential for using large sets of data to evaluate statistical populations such as the average aromatic CC bond length is best accomplished by mining crystallographic data. Biochemists can clearly examine the structures of amino acids to evaluate their zwitterionic nature. In Advanced Inorganic courses, examining molecular structure is particularly relevant. For example, the hexachlorotellurate ion has seven electron domains but has an octahedral VSEPR geometry. Main group VSEPR structure can be nicely juxtaposed with the d-block complexes with structures consistent with the Kepert model. The presentation will also discuss the delivery of an undergraduate course in practical X-ray crystallography. The course uses the crystallographic story arc as a means to have students reexamine their understanding of topics like stereochemistry and to better appreciate the process of scientific publication.

Keywords: education, crystallographic, information

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Chemical crystallography for undergraduate research: unexpected and fruitful results

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Research chemists at large academic institutions benefit from a wide range of in house chemical analysis tools and techniques. No chemistry department with a serious graduate research program would, for example, survive without mass spectrometry or nuclear magnetic resonance spectroscopy (nmr). However, at smaller, predominantly undergraduate institutions, adequate compound characterization is one of the most challenging aspects of running a research program. Techniques as "exotic" as polynuclear nmr or routine chemical crystallography are not always available, and collaboration with large universities for access to such instrumentation is vital. Here we discuss some examples of our work with Northern Arizona University (Flagstaff, AZ) and Millersville University (Millersville, PA), with whom we have provided crystallographic support for research in which all compounds are synthesized and crystallized by undergraduate or high school students. We will focus on how unexpected crystallographic results were used to rationalize the chemistry, and drive chemical research in a new direction.

Keywords: inorganic, coordination, sandwich

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Development of educational environment and student's life strategies

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The theory and practice of creating the required educational environment relating to teaching of crystallography is discussed aimed at effective growth of professional activity of science students.

It has been suggested by us and described a model (including transformation stages) of professional activity. This factor-analytical model has certain similarity with the Five-Factor Model (Big-FFM) theory, which is widely used in various applications in psychology, including description of psychobiological and social systems and fundamental works, connected with broader fundamental concepts of science, describing space-time and energetic aspects providing positive both state and development of personality.

The experimental data (groups of students involved in chemistry, geology and physics) on the role of the environment (educational, professional, natural) in instructor-student interactions are considered based on eco-psychological approach [1]. Among the two types of interaction with the environment are a subject-object and subject-to-subject interactions. As a result of their corresponding changes it is observed the emergence of positive personal growth, formation of an active, more conscious and clear life strategy. This process occurs both on a gradual basis and spontaneously. In today's rapidly changing world the actual result of obtained education is to assist formation of a specialist who is able to continuously improve self-development. The experience spontaneous transitions (flash of inspiration), described as self-organizing process, is also important for this.

Realization of the task of creation of educational environment is based on the known psychological and didactic principles of ensuring of educational environment for a better self-organization structure of student's personality. Among them are psychological principles in cooperative interaction, interactive lectures for instructors [2], involvement of students in research at an earlier stage, conscious goal-setting and awareness of ethical principles, i.e. a system of values for positive development.

The factor analysis has shown that their realization contributes to the growth of conscious personal position of a student, the development of personality and professionalism. The criteria of optimal life strategy and educational environment have been revealed, which make educational process more effective. It is noteworthy that many of crystallography concepts constitute an integral part of curriculum for many students involved in chemistry, physics, biology and material science. Therefore successful mastering of the crystallographic concepts and complex computer programs by the students can provide additional motivation and opportunity to begin a career of a scientist also.

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Keywords: educational environment, transformation, self-organizing development

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Fibre bundle approach to spin glass state and other magnetic structures with their symmetries

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The fibre bundle approach has been applied to derive the explicit formulas presenting all the eight fundamental magnetic structures and their symmetry groups, i.e. ferromagnetic, antiferromagnetic, simple spiral, ferromagnetic spiral, skew spiral, transverse spin wave, longitudinal spin wave and spin glass [1], [2]. The explanation of the uniqueness of the spin glass state has its roots in the appearance of the probability function p(i,j) in the second term of the assumed Hamiltonian. This term actually describes the random distribution of either dopants or defects in the ferromagnetic matrix under the percolation threshold. On this basis the Gaussian type randomness was derived for both the general global magnetic coupling constant and the magnetization vector, the latter effect bringing to the statistical features of the magnetic structure and the magnetic symmetry group of the spin glass state.

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Keywords: spin glass state, magnetic structure and symmetry, fibre bundle approach