

MS06.P09*Acta Cryst.* (2011) **A67**, C254**A comparative DFT study of the physical properties of a 1,2,4-triazole compound**Muhammed Dincer, Namik Özdemir, *Department of Physics, Ondokuz Mayıs University, 55139, Samsun, (Turkey)*. E-mail: mdincer@omu.edu.tr

The 1,2,4-triazole moiety is associated with diverse pharmacological activities, such as antibacterial, antifungal, antiviral, anti-inflammatory, anticonvulsant, antidepressant, antihypertensive, analgesic, and hypoglycemic properties [1]. Furthermore, some of the complexes containing 1,2,4-triazole ligands have rather peculiar structures and specific magnetic properties [2].

The experimental geometry obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations in the gas phase and in solution phase. In addition, proton transfer reactions and hydrogen bonding interactions have been studied. The solvent effect has been investigated by Polarizable Continuum Model (PCM) [3] method using three kinds of solvent (chloroform, methanol and water). Theoretical calculations were performed by means of GAUSSIAN 03W [4] at the density functional theory (DFT/B3LYP) [5,6] level using the 6-311++G(d,p) basis set [7,8].

[1] A.A. Abbas, N.S.A.M. Khalil, *Nucleosides, Nucleotides and Nucleic Acids* **2005**, *24*, 1353-1372. [2] O. Kahn, C.J. Martinez, *Science* **1998**, *279*, 44-48. [3] J. Tomasi, B. Mennucci, R. Cammi, *Chemical Reviews* **2005**, *105*, 2999-3093. [4] M.J. Frisch, *et al.* **2004**. GAUSSIAN03, Revision E.01. Gaussian, Inc., Wallingford CT 06492, USA. [5] A.D. Becke, *Journal of Chemical Physics* **1993**, *98*, 5648-5652. [6] C. Lee, W. Yang, R.G. Parr, *Physical Review B* **1998**, *37*, 785-789. [7] R. Krishnan, J.S. Binkley, R. Seeger, J.A. Pople, *Journal of Chemical Physics* **1980**, *72*, 650-654. [8] M.J. Frisch, J.A. Pople, J.S. Binkley, *Journal of Chemical Physics* **1984**, *80*, 3265-3269.

Keywords: crystallography, theoretical, solvent**MS06.P10***Acta Cryst.* (2011) **A67**, C254**Lattice energy minimization and lattice dynamics calculations on pharmaceutical hydrates**Jun-Wei Shen, *Mitsubishi Chemical Group Science and Technology Research Center, Inc., (Japan)*. E-mail: shen@rsi.co.jp

Lattice energy minimization and lattice dynamics calculations for four pharmaceutical hydrates [1] and the corresponding anhydrous were carried out with DMACRY [2] and compared with experimental structures and the lattice dynamic properties. The potential models used in this study included an empirically fitted isotropic exp-6 atom-atom model for different atomic types and a distributed multipole electrostatic model for the electrostatic interactions. Experimental structures from Cambridge Structural Database (CSD) were fully optimized, allowing for rigid body rotation, translation, and cell parameter changes within the symmetry constraints of the experimental space group. Calculated phonon frequencies ($k = 0$ rigid-body lattice modes) for the relaxed structures were used to compare with the measured terahertz spectra. All of minimized structures have shown good agreement with the experimental data. The calculated vibrational modes show that the phonon modes with strong intermolecular coupling between the pharmaceutical molecules and H_2O .

[1] T. Hulme, L. Sarah Price, *J. Chem. Theory Comput.* **2007**, *3*, 1597-1608. [2] L. Sarah Price, M. Leslieab, G.W.A. Welch, M. Habgood, L.S. Price, P.G.

Karamertzanis, G.M. Day, *Phys. Chem. Chem. Phys.*, **2010**, *12*, 8478-8490.**Keywords:** pharmaceutical hydrates, lattice energy minimization, lattice dynamics**MS07.P01***Acta Cryst.* (2011) **A67**, C254**IMAGINE, a quasi-Laue single crystal neutron diffractometer**Parthapratim Munshi,^{a,b} Flora Meilleur,^{b,c} Tibor Koritsanszky,^a Robert Blessing,^d Bryan Chakoumakos,^b Dean Myles,^b ^a*Department of Chemistry, Middle Tennessee State University, TN, (USA)*. ^b*Neutron Scattering Science Division, Oak Ridge National Laboratory, TN, (USA)*. ^c*Department of Molecular and Structural Biochemistry, North Carolina State University, NC, (USA)*. ^d*Hauptman-Woodward Medical Research Institute, NY, (USA)*. E-mail: munship@ornl.gov

A group of researchers from Physics, Chemistry, Biology, Biochemistry and Geological and Earth Sciences at Middle Tennessee State University, North Carolina State University, Hauptman-Woodward Medical Research Institute and Oak Ridge National Laboratory, with 13 additional participants from U.S. industry and academic facilities are strongly associated with the acquisition, installation and operation of IMAGINE at the High Flux Isotope Reactor (HFIR). The objective of the program, which received funding from National Science Foundation (NSF) in July 2009, is to develop a state-of-the-art facility and user-access program for neutron-diffraction analysis of advanced, complex and functional materials. IMAGINE will have broad scientific impact and community use, providing new tools, capabilities and methods for the analysis of light atom positions in materials that will be of interest across the diverse fields of structural biology, pharmacology, chemistry, condensed matter physics, nano-structured materials, and in environmental, biomedical and geological sciences. The instrument will enable the neutron structure of supra and macro-molecules to be determined at or near atomic resolutions (1.5 Å) from crystals with volume and within a time frame shorter than ever before.

IMAGINE will be commissioned in early 2012. Our team welcomes discussion and interaction with the community through the installation and commissioning phase of the instrument, and is excited to start working with the community to build an excellent education and science program. The presentation will give an overview of the IMAGINE project at the HFIR.

This research is supported by UT Battelle, LLC under Contract DE-AC05-00OR22725 for the U.S. Dept. Energy, Office of Science. The IMAGINE project is partly supported by the NSF under Grant No. 0922719.

Keywords: neutron, diffractometer, crystal**MS07.P02***Acta Cryst.* (2011) **A67**, C254-C255**Creation of a new generation of coherent x-ray sources**A.R. Mkrtchyan, A.H. Mkrtchyan, V. R. Kocharyan, A.E. Movsisyan, *Institute of Applied Problems of Physics NAS RA, Yerevan*. E-mail: malpic@sci.am

The effect of influence of external acoustic fields on X-ray transition radiation of relativistic electrons was first investigated theoretically [1] and experimentally [2]. These investigations showed that the acoustic field amplitude increase leads to an increase of the intensity of transition radiation.

In the present work details of experimental investigations of X-ray transition radiation from the periodical permittivity structure are discussed. It is shown the possibility of Creation of a new generation of coherent x-ray sources according the scheme presented in the Figure below.

This phenomenon is observed for electrons of 20 MeV energy. For the electrons source we used the LEA-50 linac of the Yerevan Physics Institute [2]. The beam parameters are: current of the electron beam is 0.1 mA, the energy resolution is ± 30 KeV, the vertical aperture is 0.0005 angular radian, the horizontal aperture is 0.01 angular radian. As a sample of investigations amorphous quartz with different thickness was taken. The acoustic field in the sample was excited by a specially designed system of high Q resonators. The emitted transition radiation and electron beam passes trough vacuum tube. For separation of the produced transition radiation from electron beam, additionally X-cut quartz crystal was placed after the amorphous quartz sample. The crystal was placed in the specially designed MHz mount and has satisfied full pumping condition for transition radiation [3-4]. The separated transition radiation passes trough vacuum tube and can be used as a coherent x-ray source.

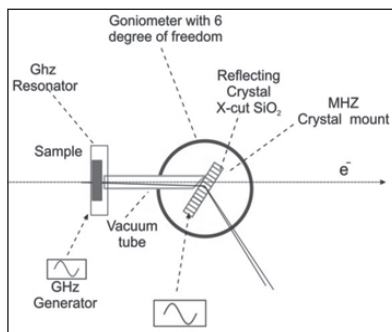
The detailed analysis of experimental data shows that the peak of intensity depends on amorphous quartz purity, frequency and amplitude of the excited hyper frequency acoustic fields.

Results of investigation shows:

- The intensity of radiation may be varied by changing the value of hyper frequency electromagnetic field amplitude.
- The registered value of ratio N_T/N_e is very large from expected and depends on target quality.
- The intensity of the radiation depends of $\Delta\omega_s$ (i.e. boundary layers of plots by $\Delta\omega_s$).
- The analysis of numerous experiments results shows that the ratio value varies in the range > 1 .
- For the targets of different summary thickness the intensity has no changes, i.e. only last layers have contributing in intensity.

According to the developed theory [1] the estimation of measured parameters has been in good agreement.

Let us note also that as a source of monochromatic x-ray radiation it can be used PXR when the crystal is excited by acoustic field.



[1] A.R. Mkrтчyan et al. Preprint ASA SSR, IAPP, Yerevan **1987**. [2] A.R. Mkrтчyan et al. Nanotechnologies in the area of physics, chemistry and biotechnology, Fifth ISTC SAC, Seminar. St. Petersburg, Russia, **2002**, 202-204. [3] A.R. Mkrтчyan et al. Письма в ЖТФ. **1983**, 9, 19, 1181-1184. [4] A. R. Mkrтчyan et al. *Proceedings the 51st Workshop of the INFN*, Channeling **2008**, 25- 1, Erice, Italy 306-308.

Keywords: transition, radiation, X-ray

MS07.P03

Acta Cryst. (2011) **A67**, C255

Pair of canted undulator MX beamlines proposed for NSLS-II
L.E. Berman,^a M. Allaire,^a M. Chance,^b W. Hendrickson,^c A. Héroux,^a J. Jakoncic,^a Q. Liu,^c A. Orville,^a H. Robinson,^a D. Schneider,^a W. Shi,^b A. Soares,^a V. Stojanoff,^a D. Stoner-Ma,^a M. Sullivan,^b R.

Sweet,^a ^a*Brookhaven National Lab, Upton, NY 11973, (USA).*
^b*Case Western Reserve U, Cleveland, OH 44106, (USA).* ^c*Columbia U and New York Structural Biology Center, New York, NY 10032, (USA).* E-mail: berman@bnl.gov

We describe a concept for x-ray optics to feed a pair of macromolecular crystallography (MX) beamlines which view canted undulator radiation sources in the same storage ring straight section. This has been proposed for the National Synchrotron Light Source –II (NSLS-II) and can be deployed at other low-emittance third-generation synchrotron radiation sources where canted undulators are permitted.

The concept adopts the beam-separation principles employed at the 23-ID (GM/CA-CAT) beamlines at the Advanced Photon Source, wherein tandem horizontally-deflecting mirrors separate one undulator beam from the other, following a double-crystal monochromator. The scheme described here would deliver the two tunable monochromatic undulator beams to separate endstations that address different and somewhat complementary purposes, with further beam conditioning imposed as required. A downstream microfocusing beamline would employ dual stage focusing for work at the micron scale and, unique to this design, switch to single stage focusing for larger beams. By contrast, the upstream beamline would only employ single stage focusing with variable focal length.

The final x-ray hutch in the downstream position would be relatively long ($> \sim 15$ m), designed to accommodate a flexible secondary microfocusing optics system. This would include an adjustable secondary source aperture toward the upstream end of the hutch, and then microfocusing mirrors or lenses positioned just before the focus point at the experiment. When one requires the minimum beam size (~ 1 μ m or less), two-stage horizontal focusing can be pursued by adjusting the curved figure of one of the upstream horizontally-deflecting mirrors to focus the beam at the secondary source aperture. The subsequent microfocusing optics would then re-focus the beam diverging from there. When a larger beam size (10-20 μ m or greater instead of 1 μ m) having less horizontal divergence (0.1 μ rad instead of 1 μ rad) is preferred, the microfocusing optics stage can be bypassed and the focal length of the upstream mirror can be adjusted accordingly.

A challenge that will be addressed in this beamline will be the manipulation of samples to take advantage of a 1 μ m beam.

The other beamline, located upstream and with a somewhat shorter x-ray hutch ($< \sim 10$ m), would contain a more conventional beam focusing optics system (demagnifying Kirkpatrick-Baez [K-B] mirror system) that would be permanently deployed. To employ the beam effectively, even with space restrictions in this experimental hutch owed to the presence of a beam tube passing through it to deliver a beam to the downstream beamline, we plan that the operation of this beamline will be highly automated with a minimum of manual access needed.

On this beamline, it is intended that the K-B mirrors can rapidly adjust their focal lengths to tailor the beam properties according to experimental requirements.

This work is supported by the US DOE, the US NIH, and the New York Structural Biology Center.

Keywords: synchrotron_radiation_crystallography, synchrotron_radiation_optics, synchrotron_radiation_sources

MS07.P04

Acta Cryst. (2011) **A67**, C255-C256

Multilayer optics for novel sources In X-ray analytics
A. Kleine, B. Hasse, J. Graf, U. Heidorn, S. Kroth, F. Hertlein, J. Wiesmann, C. Michaelsen, *Incoatec GmbH, Max-Planck-Strasse 2, 21502 Geesthacht, (Germany).* E-mail: kleine@incoatec.de