MS06.P09

Acta Cryst. (2011) A**67,** C254

A comparative DFT study of the physical properties of a 1,2,4-triazole compound

Muharrem Dinçer, Namık Özdemir, *Departament 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, antiinflammatory, 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). Thoretical 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) A**67,** 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 DMACRYS[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 ($\boldsymbol{k}$ = 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) A**67,** 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]Departament of Chemistry, Middle Tenessee 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) A**67,** 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.