

P08.07.58*Acta Cryst.* (2008). A64, C436**Atomic displacement parameters based on quantum mechanical treatment of anharmonic oscillator**

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Gram-Charlier expansion (GCE) and one-particle potential generalized by Tanaka & Marumo (GOPP) sometime produce probability density function (PDF) with negative area which is not accessible physically. We derived atomic displacement parameters (ADPs) based on PDF without negative area, using quantum mechanical treatment of anharmonic oscillator. The ADPs including anharmonic vibrations of atoms is formulated taking the anharmonic potential as a perturbation to the harmonic potential in the 3D harmonic oscillator case. Since the first order correction to wave function of the atomic vibration is expected to be a linear combination of the wave functions of the harmonic oscillator, which is expressed in terms of Gauss-Hermite polynomials multiplied by Gaussian. In order to show it clearly the PDF functions assumed in GOPP, GCE and the present study are summarized below: GOPP $\text{Pdf}_{\text{harm}}(a + \sum d_{ijk} u_{ijk} + \sum e_{ijki} u_{ijki})$, GCE $\text{Pdf}_{\text{harm}}(1 + \sum d_{ijk} \text{He}(u)_{ijk} + \sum e_{ijki} \text{He}(u)_{ijki})$, Present $\text{Pdf}_{\text{harm}}(a + \sum b_i H(u)_i + \sum c_{ij} H(u)_{ij} + \sum d_{ijk} H(u)_{ijk} + \dots)^2$. Where He or H denotes Chebychev-Hermite or Gauss-Hermite polynomials. The three methods commonly assumed that each atom vibrates independently from others. Since the squares of the wave function is the PDF function of the atom, PDF function never be negative in the present study, while in the other methods it easily becomes negative. Since the formalism of the present study is based on the quantum mechanical treatment of vibration, it is expected to represent the ADPs of X-ray diffraction more properly than GCE. Since recent development of neutron diffraction like J-PARC project will increase the opportunity to get more reliable ADPs, the ADP formalism becomes more important and can be compared on more reliable experimental facts.

Keywords: probability density function, atomic displacement parameters, anharmonic oscillator

P08.08.59*Acta Cryst.* (2008). A64, C436**Amoxicillin trihydrate - potassium clavulanate solid solution**

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Amoxicillin trihydrate and potassium-clavulanate for several decades have been combined in a drug dosage form to maintain amoxicillin's antibiotic potency. In fact, the high variability quality and pharmacokinetic profile of their dosage forms often found. This phenomenon was predicted base on their solid state intermolecular interaction. Then, the investigation of this interaction were performed by crystallography analyzes, such as thermal analysis, Powder X-Ray Diffractometer, Scanning Electron Microscope, Fourier Transformed Infra Red, and Neutron Magnetic Resonance. A series of amoxicillin-clavulanate molar fractions were treated by freeze drying, co-ground by solvent dropping, and co-heating. Crystallographic data proved that amoxicillin-clavulanate arranged a non-stoichiometrical co-crystal, known as solid solution, with the lowest energy interaction

of 1:1 molar ratio. The result of FTIR and NMR analysis depicted that the bonding was occurred between amine of amoxicillin with the carboxylic of clavulanate and also hydrates of amoxicillin with amine and carboxylic of clavulanate. Furthermore a salt reaction arranged after freeze drying. The solid solution showed different physico-chemical properties and antibiotic potency compare to each single component and their physical mixture counterparts.

Keywords: intermolecular interaction, solid solution, amoxicillin-clavulanate

P08.08.60*Acta Cryst.* (2008). A64, C436**Cohesion forces in halomethane crystals**

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Methanes are the simplest carbon compounds and therefore their structures are of fundamental interest. The methane molecules interact by van der Waals forces, and owing to the small size and bulky shape the close packing of molecules is not severely restricted by close packing in the crystal structures [1]. In this respect methanes can be considered as models for the aggregation of molecular fragments in many organic substances. An analogous reasoning applies to halogenated methanes, however their structures additionally reveal the basic aggregation patterns involving halogen...halogen and CH...halogen contacts. Along with hydrogen bonds, halogen...halogen interactions are considered to be the strongest of cohesion forces in molecular crystals, but their role for molecular aggregation is still disputable. Apart from the evidence of molecular attraction to the halogen atoms, there are also arguments for their repulsion. Hence we have studied a series of halomethanes [2-4]. Isostructural relations and phase transitions of halomethanes have been rationalized by the competing patterns of CH...halogen hydrogen bonds and halogen...halogen intermolecular interactions. The obtained results shed new light on the nature of these intermolecular interactions and on the values of van der Waals radii in molecular crystals [5].

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Keywords: intermolecular interactions, high-pressure structures, halogens

P08.08.61*Acta Cryst.* (2008). A64, C436-437**Structural studies of CLIC protein complexes**Juanita Mintono Phang¹, Stephen J Harrop^{1,2}, Krystyna E Wilk¹, Anthony Duff³, Samuel N Breit², Paul MG Curmi^{1,2}¹University of New South Wales, Biophysics, School of Physics, University of New South Wales, Sydney, New South Wales, 2052,