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Acta Cryst. (2011) **A67**, C376**The crystal structure of a short alkyl chain pyridine-based bisurea compound**

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The crystal structure of 2,6-Di(ethylurea)pyridine (EUPy) has been determined by X-ray diffraction method. The asymmetric unit comprises of one crystallographically independent molecule of EUPy, while the unit cell consists of four molecules of EUPy.

The self assembly phenomena in EUPy is driven by strong hydrogen bonds. The hydrogen bonding network suggests that one of the N-H groups in the urea moiety (N2-H4) interacts with O1 in a self assembly fashion and the other N4-H6 forms hydrogen bond with nitrogen of the pyridyl moiety through an intramolecular interaction, while in the other urea moiety both N-H groups (N3-H5 and N5-H7) form bifurcated intermolecular hydrogen bond with O2.

The molecular packing of EUPy exhibits a layered structure. Within each layer, the adjacent chains run parallel with an interchain distance of 12.95 Å producing zig-zag or wave-like structure in the *ab*-plane. The neighboring layers are almost orthogonal to each other and do have interlayer spacing distance of 7.14 Å. The orientation of the pyridine rings changes in the layer. The packing fashion of the alkyl chains are dependent on the directionality of the hydrogen bonds.

Keywords: functional materials, bisurea gelators

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Acta Cryst. (2011) **A67**, C376**A synthon-based approach to generating a solid crystalline form of propofol**

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Crystal engineering and cocrystal design of active pharmaceutical ingredients (APIs) are currently of interest in the pharmaceutical industry due to the associated possible improvement of API properties [1]. Presented herein is a crystal engineering strategy for the anaesthetic propofol (2,6-diisopropylphenol) (PRO), based on prior knowledge of relevant complementary hydrogen-bonded supramolecular synthons. PRO – a liquid at room temperature with very low aqueous solubility [2] – has been cocrystallised in a 1.5:1 ratio with isonicotinamide (INC); a pharmaceutically acceptable cocrystal former [3]. Stoichiometric equivalents of PRO and INC were ground at room temperature to produce the novel, pure-phase, polycrystalline complex, with no solvent required as a reaction medium. The complex was also grown as single crystals, utilising PRO as both a reactant and a solvent. The crystal structure reported here has been solved using single crystal X-ray diffraction, revealing a structure composed of PRO...INC hydrogen bonded, one dimensional ribbons that confirm the success of the design strategy. A dual powder and single crystal variable temperature X-ray diffraction study identified a number of phase transformations in the system on cooling from room

temperature to 123K. The crystal structures of the different forms are presented and are typified by crystal symmetry changes within the PRO:INC complex. Preliminary characterisation of the complex has shown an enhancement of the intrinsic aqueous dissolution rate of PRO (compared to raw liquid PRO) as a direct result of the crystal engineering strategy.

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Acta Cryst. (2011) **A67**, C376**Towards charge-density analysis of high-pressure molecular crystal structures**

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One of the requirements for traditional charge-density analysis is the availability of high-resolution diffraction data, typically better than $1.0 \sin\theta/\lambda$. This enables the deconvolution of electron density from thermal motion. It was recently demonstrated that “normal” resolution data, $0.66 \sin\theta/\lambda$, can also be amenable to a charge-density study: by fixing atomic positions and anisotropic displacement parameters (ADPs) to values derived from an invariom refinement, which uses aspherical scattering factors, the multipole parameters can be freely refined without compromising the data to parameter ratio [1]. A better and more elegant procedure for the treatment of ADPs consists of fixing them to values calculated independently and completely *ab initio* [2].

We have taken this a step forward and here show that a careful application of the procedure enables the determination of the charge density from high-pressure data collected in a diamond-anvil cell. Previous attempts were based on a monopole-kappa refinement [3] or a maximum entropy method (MEM) approach [4]. Whilst pushing the limits of charge-density research, our procedure allows the comparison of experimentally derived properties, *e.g.* bond topological indicators, electrostatic potential and dipole moment, for high-pressure molecular crystal structures.

We use single-crystal synchrotron data, which are 60% complete to a maximum resolution of $0.63 \sin\theta/\lambda$, for a novel high-pressure polymorph of the small molecule propionamide. The charge density and derived properties for the high-pressure polymorph are compared to those of the ambient-pressure modification, for which a full charge-density analysis has been carried out.

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