interactions and crystal packing motifs.
1 Boldyreva, E. V., Acta Cryst. 2008, A64, 218-231.
2 Fabbiani F. P. A.; Pulham, C. R. Chem. Soc Rev. 2006, 35, 932-942.
3 See for example: Moggach, S. A.; Marshall, W. G.; Parsons, S. Acta Cryst. 2006, B62, 815-825; Allan, D. R.; Clark, S. J. Phys. Rev. B: Condens. Matter Mater. Phys. 1999, 60, 6328－6334.

Keywords: high-pressure polymorphism, crystal growth from solution, antibiotics

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Behaviour of the azido group in crystal structure of the intermediates of aminoglycoside antibiotics

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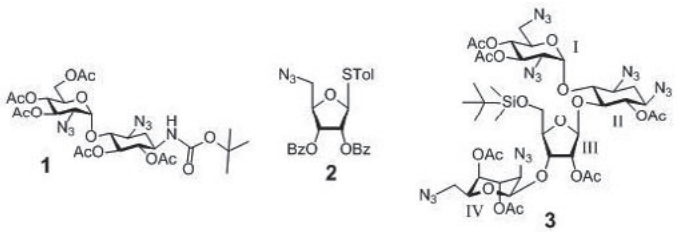
Aminoglycoside antibiotics are function through binding to specific sites in prokaryotic ribosomal RNA and affecting the fidelity of protein synthesis. Compounds **1-3** are the precursors of new derivatives of neomycin B and paromomycin. Conformational disorders of the azide groups at these compounds were observed. Compound **3** consists of pyranose (I and IV), furanose (III) and an aminocyclitol (II) rings joined together via glycosidic linkages. Compounds **1** and **2** are smaller by the number of the rings and of the azide groups. All azido groups are in a linear arrangement. In **2** it has usual geometry. The azide groups in **1** and **3** are significantly disordered. In **1** one of the azide group gave the ratio of 0.65:0.35 between the two positions, which lead to a significant distortion from the linearity. In **3** at least three from the six N_3 groups are disordered: in two the ratio between two possible conformations are 0.60:0.40 and in one- 0.80:0.20. For all of them the N=N=N angle is smaller than the literature value and most of the N=N bonds are shorter than usual bonds. Such a flexibility of the azido groups suggests that they are present in two resonance structures N=N=N and N-N≡N.



Keywords: difficult structures, antibiotics, azides

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Crystallography of steroids: A comparative analysis of geometrical features and hydrogen bonding

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Steriods are a class of biologically important organic compounds which have extensively been studied crystallographically for the last over fifty years. In view of the striking properties as exhibited by this class of materials, we have classified the cholestane (C27) into four types, viz. cholane, pregnane, androstane, oestrane, etc. and have carried out a detailed study on each of its classes to (i) compare selected bond distances and angles and their deviations from the accepted values vis-a-vis the substitutional group and X-H...A intra and intermolecular interactions, (ii) study asymmetry parameters and the importance of hybridization and ring fusions for the conformation of individual ring systems, (iii) investigate the incidence and role of X-H...A intra- and intermolecular interactions in molecular entities of this kind, (iv) prepare a database on d(H...A), D(X...A) and theta(X-H...A) range based on the cut-off criterion as proposed by Desiraju(1999), (v) study the effect of solvent on the properties of steriodal molecules and investigate the solvent-solute/solute-solvent and solvent-solvent interactions in a hydrogen bonded network. Some part of the work has been published in Acta Cryst B 2007, Z.Kristallographie, 2007., Journal of Chemical crystallography, 2007., Ind. J. Biochemistry and Biophysics 2007. A comprehensive presentation of the entire work will be made.

Keywords: crystallography, steroids, molecular structures

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Crystal and molecular structure of the diethyl ester of rhodoporphyrin

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Natural product plant porphyrins are a relatively underrepresented class in the structural databases. The current work reports the crystal and molecular structure of ethyl 8,13-diethyl-18-ethoxycarbonyl-3,7,12,17-tetramethylporphyrin-2-propionate (the diethyl ester of rhodoporphyrin) isolated from the leaves of the Thai traditional medicine plant, *Bridelia ovata* Decne, also commonly called *maka* in Thai. The structure determination was straightforward with a minor disorder of one ethyl group (refined occupancy ratio 0.77(1):0.23). The ethoxycarbonyl group is fixed to be coplanar with the porphyrin core by a concerted group of five intramolecular C－H···O interactions, while the ethyl propionate groups are oriented perpendicular to the porphyrin cores forming ribbons of intra- and inter-molecular C－H···O interactions. The other dominant packing feature is π···π stacking of the porphyrin planes, which are required to be parallel by symmetry. Experimental Data: From the leaves of *Bridelia ovata* Decne; intense violet plate crystals, recrystallized from hexane-dichloromethane solution; MP 194-196 ℃ . Crystal data: $C_{36}H_{42}N_4O_4$, *Mw*=594.74; 0.4 x 0.3 x 0.05 mm; triclinic *P*－1 (No. 2), *a*=9.409(2), *b*=12.589(2), *c*=14.683(2) Å, α=103.19(2), β=107.49(2), γ=103.40(2)°, *V*=1528.3 Å^3; *Z*=2, μ_{Cu}=0.68 mm^{-1}; d_{calc}=1.292 Mg m^{-3}; *T*=113 K; R_1(F)=0.084, *gof*=1.12.

Keywords: porphyrin, supramolecular structure, natural product

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Potassium salts of some ribonucleotides: AMP, IMP, CMP and UMP

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