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Keywords: cocrystal, incommensurate modulated structure

FA4-MS26-P20

Fluconazole and its cocrystals with maleic and glutaric acids. Ivan Leban[a], Nina Lah[a], Žiga Hodnik[b], Danijel Kikelj[b], Jože Kastelic[c] ,[a]*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, SI-1000 Ljubljana, Slovenia,* [b]*Faculty of Pharmacy, University of Ljubljana, Aškerčeva 7, SI-1000 Ljubljana, Slovenia,* [c]*Krka, d. d., Novo mesto, Šmarješka c. 6, SI-8501 Novo mesto, Slovenia.*
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Fluconazole (2-(2,4-difluorophenyl)-1,3-bis(1H-1,2,4-triazol-1-yl)-propan-2-ol), is a bis-triazole antifungal drug used to treat invasive infections caused by *Candida*. The drug is available in both oral and intravenous formulations. The crystal structures of three unsolvated forms, designated as polymorph I, II and III, as well as the structures of a monohydrate and the solvates containing ethyl acetate, acetone and benzene have already been reported [1],[2]. Here, the single-crystal X-ray structures of fluconazole (form III) and its cocrystals containing maleic and glutaric acids will be presented.
Fluconazole (III): triclinic, P-1, a=7.4907(10), b=7.7640(10), c=11.9547(10) Å, α=85.012(8), β=84.507(8), γ=75.553(8) °.
Fluconazole with maleic acid: $[(FluH_2)(Hmal)_2(H_2mal)]$, triclinic, P-1, a=5.4983(5), b=13.8723(16), c=18.433(3) Å, α=98.062(8), β=91.748(8), γ=95.479(8) °.
Fluconazole with glutaric acid: $[(Flu)(H_2glu)]$, triclinic, P -1, a=5.6897(10), b=10.6593(15), c=17.063(3)Åα=72.909(8), β=84.453 (8), γ=80.863(8) °.

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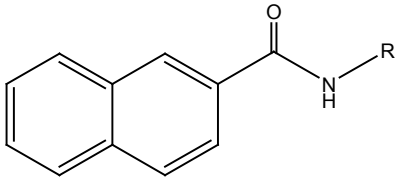
Keywords: fluconazole, maleic acid, glutaric acid

FA4-MS26-P21

Crystal packing in a series of N-phenyl-2-naphthamide derivatives. Jim Simpson[a], Aamer Saeed[b], Rasheed Ahmad Khera[b], [a]*Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, 9054 , New Zealand,* [b]*Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan*

Structures of seven N-phenyl-2-naphthamide derivatives



R = C_6H_5—, *p*—Cl—C_6H_4, *p*—CH_3—C_6H_4, *m* and *p*—CH_3O—C_6H_4, *o*—NO_2—C_6H_4 and C_6H_{10} have been determined and their crystal packing investigated. The pervasive intramolecular contact in all but one of the compounds involves classical N—H...O hydrogen bonding leading to the formation of C(4) chains [1]. The exception is the nitro derivative where a strong intramolecular N—H…O contact to an O atom of the *o*-NO_2 substituent takes precedence. Additional $C_{aromatic}$—H…O contacts support the formation of chains in some molecules with additional C_{methyl}—H…O interactions in the methoxy derivatives. C—H…π interactions occur in the majority of compounds but surprisingly, despite the presence of the planar naphthyl synthon, significant π…π stacking interactions are observed only for the nitro-derivative.

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Keywords: N-phenyl-naphthamides, structure, packing

FA4-MS26-P22

Highly Interpenetrated Organic Networks formed by Halogen Bonding Giancarlo Terraneo[a,b], Gabriella Cavallo[a], Pierangelo Metrangolo[a,b], Tullio Pilati[c], Giuseppe Resnati[a,b,c] , [a]*NFMLab - D.C.M.I.C. "Giulio Natta", Politecnico di Milano, Via L. Mancinelli 7, 20131 Milan, Italy,* [b]*CNST - IIT@POLIMI, Politecnico di Milano, Via G, Pascoli 70/3, 20133 Milan, Italy,* [c]*C.N.R. - I.S.T.M., University of Milan, Via C. Golgi 19, 20133 Milan, Italy*
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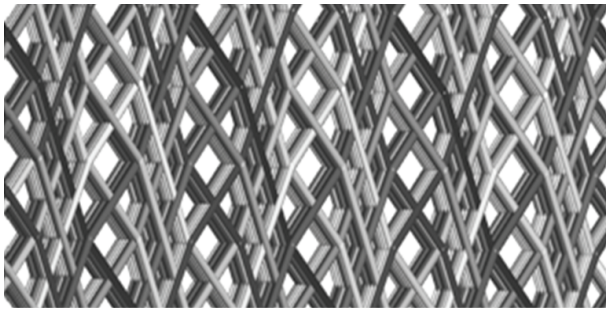
Halogen bonding (XB) [1], namely the noncovalent interactions wherein halogen atoms function as electrophilic species, can be described by the general scheme D···X-Y where X is the electrophilic halogen atom (Lewis acid, XB-donor), D is a neutral or anionic donor of electron density (Lewis base, XB-acceptor), and Y is carbon, nitrogen, halogen, etc. Recently, XB has proven its efficiency and reliability in the design and construction of self-assembled systems with quite different architectures and properties [2]. New aggregation processes can be realised, the novelty coming from either the molecular identity of assembled modules or from the way the modules are arranged in the supramolecular architecture. In this communication we describe the deliberate construction of highly interpenetrated organic networks. The focus will be on tetradentate tectons. In particular, we will show that DAB-*dendr*-$(NHC_6F_4I)_2$ self-assembles with (*E*)-1,2-bis-(4-pyridyl)-ethylene thanks to multiple N···I interactions that drive the formation of a supramolecular architecture composed of 2D square networks with a mode of interpenetration of class Ia. We will show that not only tetradentate XB-donor tectons, but also tetradentate XB-acceptors (*e.g.* tetrapyridyl pentaerythritol or cyclobutane derivatives) give rise to highly interpenetrated organic networks (Figure) [3].



Schematic view of the overall 10[5x2]-fold interpenetration of class IIIa

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Keywords: Halogen Bonding, Molecular Assemblies, Interpenetrated Networks

FA4-MS26-P23

The co-crystallization of trimethoprim with glutarimide derivatives by means of molecular recognition.

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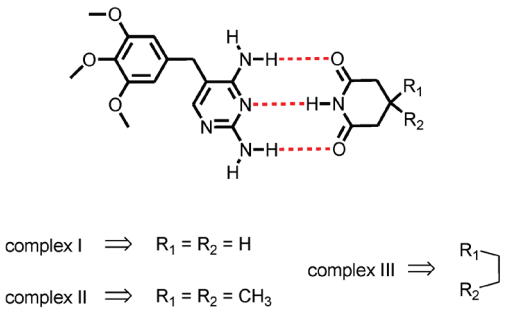
Trimothoprim is an API which is used against bacterial infections and inhibits dihydrofolate reductase [1]. It shows the necessary donor/acceptor groups for the complexation with glutarimide derivatives which have been selected for co-crystallization experiments because of their structural similarity with barbiturates [2].
1:1 co-crystals between trimethoprim and three glutarimide derivatives (glutarimide [I], 3,3-dimethyl glutarimide [II] and 3,3-tetramethylene glutarimide [III]) have been successfully synthesized. All these complexes show the expected hydrogen-bond pattern (ADA/DAD with A = acceptor and D = donor). Additional N-H…N hydrogen bonds between trimethoprim molecules lead to a diverse arrangement in the crystal packing. Complex I crystallized in $P2_1/n$ with one complex in the asymmetric unit while complexes II and III crystallized in *P*-1 with one and two complexes in the asymmetric unit, respectively. The structure of complex I is characterized by the formation of rings between two complexes (generated by inversion) through N-H…O (methoxy) interactions [$R_2^2(20)$ring in graph-set notation]. The ring units are further interlinked with each other by N-H…N hydrogen bonds. The complexes II and III show similar hydrogen-bond interactions and crystal-packing arrangements. In both cases three classical hydrogen bonds connect the glutarimide with the pyrimidine-2,4-diamine fragment of trimethoprim. These complexes are centrosymmetrically bridged through a pair of N-H…N hydrogen bonds, involving the two amino groups and the pyrimidine ring nitrogen. A thorough analysis of the hydrogen bonds in each crystal as well as the differences and similarities in the crystal packing within these three complexes will give insight into the design of co-crystals. Furthermore, a comparison of the conformations of trimethoprim in different structural environments demonstrates its conformational flexibility [3].



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Keywords: API, co-crystals, hydrogen bonds

FA4-MS26-P24

Molecular interactions in complexes of 4,4'-Dinitrobiphenyl.

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The focus of this study was to investigate the nature of molecular donor-acceptor interactions in the solid state, using spectroscopic techniques such as IR, Raman, NMR and X-ray crystallography. Complexes of para disubstituted and 4-monosubstituted biphenyl formed with 4,4'-dinitrobiphenyl (DNBP), demonstrate intense colours, from pale yellow to dark red, upon formation. These colours are dissimilar to the colour combination of the parent compounds. Typical interactions observed in such molecular complexes include π-π interactions, hydrogen bonding, charge transfer and van der Waals interactions. Complexes of DNBP, as the host molecule, included a variety of mono- and disubstituted biphenyl donors or guests, such as dihalo, diamino, di- and monohydroxy groups[1], as well as urea with a 1:1 host:guest ratio [2] and thiourea with a 7:6 ratio. Molecular complexes formed between DNBP with difluorobiphenyl with a 3:1 ratio and DNBP with dibromobiphenyl and diiodobiphenyl, both with 4:1 ratios, showed similar packing styles. The crystal structures of these complexes showed retention of the non-planar conformation of DNBP with a dihedral angle between the phenyl rings of around 35^{O}[3]. However, the dihedral angle between the phenyl rings of the diflouro-, diiodo- and dibromobiphenyl in these complexes indicate that these guests are essentially planar. The conformation for DNBP has also been confirmed using density functional theory (Guassian03) calculations that showed good agreement between the theoretically calculated and experimentally observed IR and Raman spectra in the solid state. It appears as if the packing of the complexes in the solid state is directed mainly by the similar packing of DNBP units in these complexes. Some of the molecular ratios for these complexes that vary, depending on the electronic properties of the donor molecules, were determined using NMR spectroscopy.

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