**PS05.07.02 STRUCTURAL SYSTEMATICS OF MYO-INOSITOL DERIVATIVES.** Carl H. Schwabé & Ian D. Spiers, Pharmaceutical Sciences Institute, Dept. of Pharmaceutical & Biological Sciences, Aston University, Birmingham B4 7ET, U.K.

Myo-inositol 1,2,3-trisphosphate may act biologically as an ion channelator and anti-oxidant. While developing an efficient synthesis of this biochemical we obtained crystal structures of four key intermediates, the final product, and a related derivative of myo-inositol (MI):

1. D/L-1,2,4,5-di-O-cyclohexyldiene MI
2. D/L-1-O-(t-butyldiphenylsilyl)-2,3-O-cyclohexyldiene MI
3. 4,5,6-tri-O-benzoyl MI
4. 4,5,6-tri-O-benzoyl MI 1,2,3-tris(dibenzyl phosphate).

Related structure determinations describe 23 independent molecules.

**PS05.07.03 SYNTHESIS AND CHARACTERIZATION OF COPPER, NICKEL, COBALT 2-FORMYLURACIL THIOSEMISCARBAZONE COMPLEXES.** G. Pelino, M.Belicchi Ferrari, G.Gasparri Fava, P.Tarasconi, R.Rossi, Dip. di Chimica Generale ed Inorganica, Chimica Analitica, Chimica Fisica e Centro di Studio per la Strutturistica Diffrattometrica del CNR, Viale delle Scienze 78, Università degli Studi di Parma, 43100 Parma, Italy

In order to elucidate the biological effects of thiosemicarbazones on Friend erythroleukemia cells (FLC), an extensive work is being carried out in our laboratory on a wide range of derivatives and their transition metal complexes systematically followed by tests in vitro. Most recently our attention has been focused on the influence of the aliphatic/aromatic nature of the ligand and the stereochrome of the metal ion on the biological activity of this class of compounds. At present we are synthesising and characterising metal complexes of a novel compound. 2-formyluracil thiosemicarbazone (H2ut). With this ligand we have recently reported the crystal structures of copper- and cobalt-containing complexes prepared starting from their divalent ions chlorides: [Cu(H2ut)(OH)2Cl]2H2O and [Co(H2ut)2]3H2O. The new compounds we are presenting have been prepared by adding HCl to Cu(NO3)2·3H2O and NiCl2·6H2O water solutions. The crystals obtained have the following stoichiometry: [Cu(H2ut)(OH)2]SO4·3H2O and Ni(H2ut)(OH)2Cl·H2O. The former crystallises in space group C2/c, with cell constants a=21.009(5), b=12.174(4), c=14.900(4) Å, β=125.44(3)°.

The copper atom presents a square pyramidal coordination geometry with the basal plane positions occupied by the ligand O,N,S atoms, the fourth position by a water and the apical position by a sulphate oxygen. The latter presents cell parameters of a=16.345(5), b=12.967(4), c=6.756(2) Å and β=92.40(1)°, space group P21/c. The nickel atom coordinates octahedrally six donor atoms: the equatorial positions are the same as the previous compound while the two apices are occupied by a water molecule and a chloride ion. The remaining charge on the metal is neutralised by a second chloride ion lying outside its coordination sphere.


**PS05.07.04 CRYSTAL STRUCTURES OF AZOLOPYRIDAZINES.** Anna Katrusiak, S. Balomiak and A. Katrusiak, Department of Organic Chemistry, Karol Marcinkowski University of Medical Sciences, Grunwaldzka 6, 60-780 Poznan, Poland; *Department of Crystal Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland

Crystal structures of several azoopyridazine derivatives will be presented, and the molecular aggregations and interactions compared and discussed. Triazolo- and tetrazoloazopyridazines show interesting biological and pharmacological activities and have been applied in various drugs [A. Deeb and S. A. Said, Collect. Czech. Chem. Commun. 55 (1990) 2795]. The pyridazine ring is a fragment of many compounds of a broad biological activity, for example bacteriostatic or cystostatic, and inhibitors in enzymatic processes [G. Biagi et al., Farmaco 47 (1992) 91]. The investigated series include 6-hydradrazino-, 6-morpholino-, and 6-azido-1,2,3,4-tetrazolo[5,4-b]pyridazines, and 6-azido-1,2,3,4-triazolo[4,3-b]pyridazine. In the crystal lattices the molecules are usually arranged into planar sheets. Short intermolecular contacts C-H...N have a character of weak hydrogen bonds, influence the molecular aggregation, and appear to be characteristic interactions in the structures of these compounds.

**PS05.07.05 CRYSTAL STRUCTURE OF A BETA-CARBOLINE DERIVATIVE - MEDICINALLY ACTIVE COMPOUND.** L.Govindasamy, D.Velmurugan, K.Ravikumar(1) and A.K.Mohanakrishnan(2), Department of Crystallography and Bio-physics, University of Madras, Madras-600 025, India; (1)Laboratory of Crystallography, Indian Institute of Chemical Technology, Hyderabad-500 007, India; (2)Department of Organic Chemistry, University of Madras, Madras-600 025, India

The use of β-carbolines has been instrumental for the development of the inverse agonist / agonist pharmacophore of the benzodiazepine receptor site(BzR). The BzR plays a central role in the molecular mechanism controlling anxiety, memory learning, sleep, convulsant and proconvulsant activities. In view of the above importance we report the crystallographic study of one of the β-carboline derivatives. Preliminary results: C25H19NO2·O2S2, P̅21bar, a=10.184(1), b=10.941(1), c=13.441(1), α=84.80(2), β=67.94(1)° and γ=82.65(2). The crystal structure was solved by Direct methods and refined to a final R value of 0.055. The conformational features will be presented.