MS20 P01

Solid state complexes of calix[4]arene diphosphate with chlorhexidine and pilocarpine. Oksana Danylyuk[a], Kinga Suwinska[a], Adina Lazar[b], Anthony W. Coleman[b],[a]*Institute of Physical Chemistry PAS, Warsaw, Poland.* [b]*IBCP, Lyon, France.*
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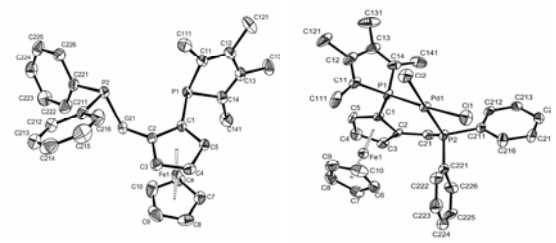
Keywords: calix[4]arene, water-soluble, co-crystal

Pharmaceutical co-crystals, formed between an active pharmaceutical ingredients (API) and a co-crystal former, have been the subject of growing interest in the last decade. The co-crystallization of drug with co-crystal former offers the opportunity to modify chemical and physical properties of API and control drug conformation. The calix[*n*]arenes are a class of macrocyclic organic host molecules widely studied due to theit ability to include a wide range of neutral and charged guests. The capacity of the calixarenes to complex various molecules in aqueous phase is interesting for biopharmaceutical application. The solid state structure of the molecular complexes of water-soluble calix[4]arene diphosphate with antiseptic chlorhexidine and dopamine agonist pilocarpine will be presented. In both cases, the drug molecules are complexed outside the macrocyclic cavity of the host due to the interdigitation of two calixarenes forming a dimeric unit. The role of hydrogen bonds and aromatic-aromatic interactions will be discussed.

MS20 P02

Design of New Chiral Ferrocene-Bridged Phosphole ligands. Sandrine Vincendeau, Eric Manoury, Maryse Gouygou, Jean-Claude Daran. *Laboratoire de Chimie de Coordination, 205 route de Narbonne, 31077 Toulouse Cedex, France.* E-mail : daran@lcc-toulouse.fr

Development of asymmetric metal-catalyzed reactions has played a significant role in allowing synthetic access to biologically important molecule. Enantiopure 1,2-disubstituted ferrocene derivatives, especially ferrocenyl-phosphine ligands, have been widely and successfuly used as ligands in homogeneous transition metal catalysis.[1] Most of these chiral ferrocene based ligands possess classical tertiary phosphine group and no attention has been paid to ferrocenyl ligands with non-classical phosphine such as phosphole.
As part of our continuing interest in the ferrocene chemistry[2] and in the design of new chiral phosphole based ligands[3], we have investigated the synthesis and X-ray structural characterization of a series of mixed phosphole-ferrocene ligands and investigated their coordination chemistry.



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MS20 P03

Synthesis, crystal structure and biological activity of the nickel(II) complex of 2,6-diacetylpyridinedihydrazone
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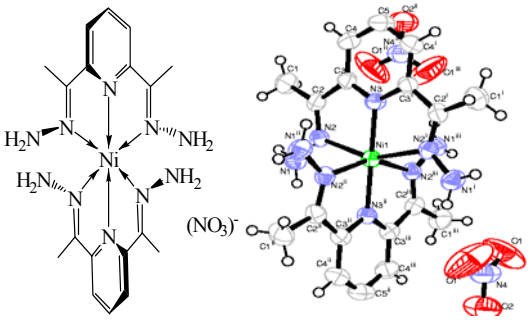
Keywords: Diffraction structure analysis, nickel(II) complex, antibacterial and antifungal activity

A complex of Ni (II) with 2,6-diacetylpyridinedihydrazone (L) towards nickel(II) has been prepared and characterized by means of elemental analyses, IR, electronic spectra and single crystal X-ray analyses. $[NiL_2](NO_3)$, was crystallized in the tetragonal space group P-4 21 c. The complex exhibits the expected coordination sphere with six nitrogen atoms coordinated to the central Ni^{II} with a deformation from pseudo-octahedral geometry. The Antimicrobial activities of the ligand and its complex were investigated.



MS20 P04

Theme and variations: the conformational polymorphs of chlorpropamide Tatiana N. Drebushchak[a,b], Nikita V. Chukanov[ac], Elena V. Boldyreva[ab], [a]REC-008 Novosibirsk State University, Russia, [b]Institute of Solid State Chemistry and Mechanochemistry SB RAS, [c]Novosibirsk Institute of Organic Chemistry SB RAS, E-mail: boldyrev@nsu.ru

Keywords: polymorphism, pharmaceuticals, crystal engineering

The problem of polymorphism of drug substances is important for several reasons. If a polymorphic transition occurs during manufacturing process, the un-controlled formation of another polymorph as compared to the starting material can result in the deterioration of the quality of a dosage form in terms of its bioavailability, or shelf-life. It can also have consequences if a patent specifies the manufacture and sale of a particular polymorph. On the other hand, an ability to control the polymorphism of a drug opens new routes to improving the quality of an already known product and to launching new products into the market.