

porphyrin complexes as sensors of spermine is reported.

[1] a) Di Costanzo L., et al., *Angew. Chem. Int. Ed. Engl.*, 2001, **40**, 4245; b) Moschetto A., et al., *J. Am. Chem. Soc.*, 2002, **124**, 14536.

**Keywords:** non covalent assembly, porphyrins, sensors

#### P.06.06.6

*Acta Cryst.* (2005). A61, C284

#### Strychnine and Brucine Self-Assemblies: Structures and Properties

Agata Bialonska, Zbigniew Ciunik, Faculty of Chemistry, University of Wrocław, Wrocław, Poland. E-mail: bialonsk@wcheto.chem.uni.wroc.pl

Strychnine and brucine self-assemblies play an important role in molecular recognition during racemic resolution by fractional resolution [1]. Different strychnine and brucine self-assemblies are accountable for their "quasi-enantiomeric" behaviour in some cases of racemic resolution [2], [3]. Change of alkaloid self-assemblies can lead to change of recognition sequence of resolved enantiomers [3].

Controlling time of crystallization, they can play an important role for determination of various sizes and topologies water cluster.

Surfaces of the strychnine and brucine self-assemblies have determined their various arrangement of chloride anions, that lead to destruction by redox reaction of only brucine molecules. The brucine sheet determines hydrogen bonds network, where chloride anion is linked to chair water hexamer (similar water-chloride anion structure is observed for ionization of HCl on ice at low temperature leading to formation of polar stratospheric clouds and further to ozone holes). Bilayer sheet of strychnine, which determines helical arrangement of chloride anions and water molecules into channels, preserves strychnine molecules from destruction.

[1] Jacques J., Collet A., Wilen S.H., *Enantiomers, Racemates and Resolutions*, Ed.: Krieger Publishing Company, Malabar, Florida, 1991. [2] Gould R.O., Walkinshaw M.D., *J. Am. Chem. Soc.*, 1984, **106**, 7840. [3] Bialonska A., Ciunik Z., *CrystEngComm.*, 2004, **6**, 276.

**Keywords:** supramolecular assemblies, recognition molecular, alkaloid structures

#### P.06.06.7

*Acta Cryst.* (2005). A61, C284

#### Polymorphism in an Anti-implantation Agent: A Subtle Interplay of Weak Intermolecular Interactions

Deepak Chopra<sup>a</sup>, K. Nagarajan<sup>b</sup>, Tayur. N. Guru Row<sup>a</sup>, *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012*. <sup>b</sup>Hikal Limited, Bannerghatta Road, Bangalore-560076. E-mail: deepak@sscu.iisc.ernet.in

Polymorphism is defined as a solid crystalline phase of a given compound resulting from the possibility of at least two crystalline arrangements of that compound in the solid state. Substituted Indol-4-ones are anti-fertility agents and have been used for the inhibition of implantation activity in rats. Polymorphism in 1-(4-fluorophenyl)-3,6,6-trimethyl-2-phenyl-1, 5, 6, 7-tetrahydro-4H-indol-4-one based on solvent variation and the subsequent changes in intermolecular interactions is discussed.

A complete analysis has been made in terms of morphology, Single Crystal Structure, Powder X-Ray diffraction, Non Linear Optical Activity (NLO) and Differential Scanning Calorimetry. Polymorph (P1) crystallizes from a solution in Dichloromethane/Hexane in a monoclinic space group, non-centrosymmetric P2<sub>1</sub> (as plates) whereas the second polymorph (P2) crystallizes from a solution in EtOH/Acetone in a tetragonal space group, centrosymmetric P4<sub>2</sub>/n (as blocks).<sup>1</sup> C-H...O and C-H... $\pi$  intermolecular interactions forming chains stabilize P1 while P2 is stabilized by C-H...O and C-H... $\pi$  dimers and a not so common F...F intermolecular interaction.

[1] Chopra D., Nagarajan K., Guru Row T.N., *Cryst. Growth & Design*, 2005, in press.

**Keywords:** polymorphism, intermolecular interactions, NLO

#### P.06.06.8

*Acta Cryst.* (2005). A61, C284

#### Morphotropism: A Link between the Similarity and Polymorphism of Organic Crystals

Alajos Kálmán, Institute of Structural Chemistry, HAS Budapest, Hungary. E-mail: akalman@chemres.hu

Kitaigorodskii, in *Organic Chemical Crystallography* (1961) – applied a term "morphotropic step" by the aid of which nonisomorphous crystals of chemically similar molecules may keep their close packing coefficient around 0.6-0.7. However, the essence of the phenomenon remained unanswered. Since 2000, an ongoing analysis of the supramolecular self-assembly of disubstituted cycloalkanes led to the discovery of nine packing patterns built up by hydrogen bonded homo- and heterochiral chains of racemic molecules, associated either antiparallel or parallel array [1]. Since every pattern is represented at least by one crystal structure (solved in Budapest), the chemical similarity and crystallographic properties of these crystals led to a recognition that these distinct patterns, by pairs, mostly differ only by one non-crystallographic turn of motifs forming a pattern, or the whole pattern turns through 180°. A proper definition of the word *morphotropism* helped to identify non-crystallographic turns with the morphotropic steps left unexplained by A.I.K. It has been shown that stereoisomers, in particular, are related by a morphotropic step, which may also play a bridge between isostructural crystals, and occasionally hallmarks the enantiotropic polymorphism of molecules. While a non-crystallographic turn between isostructures and stereoisomers is imaginary, polymorphs are linked by real, solvent mediated turns of the motifs.

[1] Kálmán A., Fábrián L., Argay Gy., Bernáth G. Cs., Gyarmati Zs., *Acta Cryst.*, 2004, **B60**, 755, and references therein.

**Keywords:** isostructurality, morphotropism, polymorphism

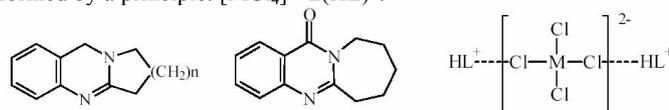
#### P.06.06.9

*Acta Cryst.* (2005). A61, C284

#### The Crystal Structural Variety of Tricyclic Quinazoline Salts

Bahodir Tashkhodjaev, Akmal Tojiboev, Kambarali K.Turgunov, Khusnuddin M.Shakhidoyatov, *S.Yunusov Institute of Chemistry of Plant Substances, Tashkent, Uzbekistan*. E-mail: rentgen@uzsci.net

Quinazoline type of alkaloids are widely distributed in plants and induce a wide spectrum of biological activity. Usually they are used in applied medicine in a form of salts. For this reason their structures have practical importance. Hydrochlorides of tricyclic 3,4-dihydroquinazolines (L) easily form complexes with chlorides of metals (M= Zn, Co, Cu). Thus crystallographic independent unit is formed by a principle:  $[MCl_4]^{2-} \cdot 2(HL)^+$ :



In salt complex of alkaloid (n=3) with ZnCl<sub>4</sub> two polymorphic crystals have been found. Crystallographic independent unit forms a skeleton. Change in geometry of this skeleton can give rise to polymorphism. Hydrochlorides of alkaloids with n=1-3 are dihydrates. Here the aqua-systems are stabilized in crystal by hydrogen and the donor – acceptor interactions.

Similar skeletons form complex chlorides of 2,3-pentamethylen-3,4-dihydroquinazolone-4 with chlorides of metals. But this skeleton includes 3 water molecules. Crystals of hydrochlorides, depending on a crystallization condition, can be hydrates (inclusion 4.5 water molecules). However, these crystals after recrystallization transform into stable hydrochlorides.

**Keywords:** alkaloid structures, supramolecular assemblies, inclusion phenomena

#### P.06.06.10

*Acta Cryst.* (2005). A61, C284-C285

#### Macrocyclic Amines and their Adducts with Acids

Teresa Borowiak<sup>a</sup>, Grzegorz Dutkiewicz<sup>a</sup>, Maciej Kubicki<sup>a</sup>, Marek Pietraszkiewicz<sup>b</sup>, Oksana Pietraszkiewicz<sup>b</sup>, Rainer Mattes<sup>c</sup>, *a*Faculty of