control of the spin crossover phenomenon. Widely studied in iron(II) molecular complexes, it can be induced by a change of temperature, pressure or by light irradiation and is accompanied by particular changes in the magnetic, optical and structural properties of a material. Intrinsic to these compounds and a 'must' for applications is their bistability, i.e. the possibility of changing between two molecular states in a controlled, reversibly and detectable manner in response to a specific perturbation. Hence, determining and studying the molecular factors that will predispose a material to undertake a spin transition, and understanding how this transition affects the resulting structure and properties, is then crucial for the designing of new materials showing enhanced properties useful for practical applications. However, when subjecting materials to a diversity of extreme sample environments, it is usual to find a variety of responses, including new and/or uncommon structural changes and features. This talk will show a few examples of structural diversity in spin crossover complexes induced by different sample environments.

Keywords: low temperature, light irradiation, high pressure

MS.28.2

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Crystal structure of 6PicTubenzo thiourea derivative, oxidative cyclization and coordinated with Cu^{2+}

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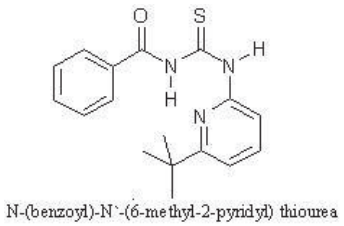
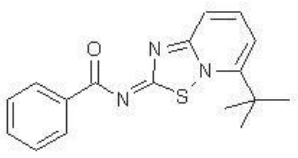
Thiocyanates (sulphocyanate or thiocyanide) are analogous to the cyanate ions. The reaction of these compounds with amine groups in the different materials form ourea and thiourea derivatives. The complexes of thiourea and thiourea derivatives are important since they have shown antitumor, antiviral, bactriostatic and antioxidative activity.[1,2] One of the interesting features of some thiourea derivatives is to be oxidized in the presence of a reductant and produce the oxidative cyclization compounds. These new compounds also act as ligands and coordinate to the metal ions.[3] In this report, at first N-(Benzoyl)-N`-(6-Methyl-2-Pyridyl)Thiourea (6picTu(Benzo)) is introduced. It is prepared from benzoyl isothiocaynate and 6-methyl-2-pyridyl. Then, (6picTu(Benzo)) reacts with the $CuCl_2$ in ethanol solution. The oxidative cyclization occurs and is generated N`-(5-methyl[1,2,4]thiazolo[2,3-a]pyridine-2-yldine)benzamide. The new complex is build by this product and $CuCl_2$. CHN, AA-, IR-, ^{1}HNMR- and ^{13}CNMR spectroscopies are used to characterize the products. The crystal structures of these compounds from suitable solvents are determined with X-ray single crystal diffraction.



N-(benzoyl)-N`-(6-methyl-2-pyridyl) thiourea



N`-(5-methyl[1,2,4]thiazolo[2,3-a] pyridine-2-yldine) benzamide

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Keywords: benzoyl isothiocyanate, benzoyl thiourea, oxidative cyclization, complexes $CuCl_2$

MS.28.3

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Synthesis and crystal structures of diorganotin schiff base complexes

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Schiff bases are known to form a wide range of coordination compounds with transition metal and main group metals. The X-ray crystal structures of three organotin Schiff base complexes were studied. One of the complexes, N,N ´ -cyclohexylenebis(salicyli deneiminato)dibutyltin(IV) dichloride crystallises in monoclinic, *C*2/*c* space group with the unit cell parameter, a = 15.0080 Å, b = 14.0472 Å, c = 14.2802 Å and β = 112.703º. The octahedral tin environment is formed by the two butyl groups and two chloride atoms from dibutyltin dichloride as well as two oxygen atoms, one from each of the adjacent N,N ´ -cyclohexylenebis(salicy lideneiminate ligand forming a polymeric chain. On the hand, N-(2-Amino cyclohexyl)(salicylaldiminato)dichlorophenyltin(IV) chloroform solvate, crystallizes in monoclinic, $P2_1/n$ with the unit cell parameter, a = 11.559 Å, b = 11.877 Å, c = 18.766 Å and β = 108.449°. The octahedral tin coordination environment is completed by a phenyl ring ,two chlorides ions , two donor nitrogen atoms and one hydroxyl oxygen atoms from the N,N'-cyclohexylenebis(salicy lideneiminate ligand; the bonded C atoms of the phenyl ring along with three chelating atoms comprise an approximate square plane. The third structure analysed is N,N ´ -4,5-dimethyl-1,2-phenylene-bis(salicylideneaminate)dicyclohexyl(IV) which crystallises in monoclinic, $P2_1/c$ space group with the unit cell parameter, a = 10.1419 Å, b = 17.2985 Å, c = 16.990 Å and β = 102.668º. The structure of this complex is also found to adopt the octahedral tin environment comprising two nitrogen donor atoms and two oxygen donor atoms from the ligand and two cyclohexyl groups. This complex differs from the previous two in that the two chlorides have been substituted by the oxygen atoms.

Keywords: diorganotin, schiff base, crystal structures

MS.28.4

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Unusual C-Br$\cdots\pi$ interactions in ferrocenyl systems

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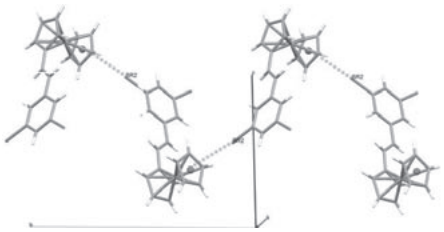
As part of our ongoing investigations into fluorescent dyad and triad systems1, we have prepared (E)-1,3-dibromo-5-(2-(ferrocenyl)vinyl) benzene as a precursor to donor acceptor compounds in which a ferrocene donor is linked via conductive alkene and alkyne bridges to fluorescent acceptors such as naphthalimides. The structure of the molecule is reported here. In the crystal structure, packing relies exclusively on C-Br...π interactions with Br...Cγ distances of 3.846(2) and 3.5983(12) Å and C-Br...Cγ angles, 168.42(9) and 171.66(8) ° respectively, where Cγ represents the centroids of unsubstituted cyclopentadiene rings of the ferrocene molecules.

These contacts link molecules into helical coils which are further aggregated to form a network structure. A database search reveals 10 ferrocenyl derivatives displaying similar contacts but only two of these depend solely on the C-Br...π interactions for structural stability.



Keywords: ferrocene compounds, crystal engineering, interactions

MS.28.5

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Unexpected patters in co-crystals of small molecules

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Acetylene is a surprisingly good candidate for co-crystallization. It is a reasonable good double proton donor and a good pi-acceptor. The small and rigid molecule is therefore expected to form easy-to-understand primary motifs in the solid state. With mono-functional small proton acceptors such as ethers, carbonyls or alcohols applied as co-crystal partners we thought to find dumbbell-like molecules and with bi-functional partners, linear chains are likely. The same is anticipated with N-containing partners like amines, amides and hetero-aromatic systems. When no acceptor atoms but pi-acceptors are available, we assume that acetylene will prefer C-H...π interactions and the formation of chains. But only a few systems obey the rules. Some of the anticipated dumbbell-like molecules are found as zigzag chains, sometimes the acetylene is mono-dentate with dangling hydrogen atoms, and often the geometry does not hold the expectations that lone pair positions are directed towards the hydrogen atoms. In most of the cases, the electrostatic character of these weak hydrogen bonds seems to dominate the geometries and the directionality is less important. Instead, the secondary interaction not only determine the packing but also the question, whether molecular complexes are found or not. Comparison of acetylene complexes with benzene and substituted benzene, e.g. mesitylene, xylene, perfluorobenzene etc. reveals interesting and varying features.

Keywords: cocrystals, hydrogen bonds in organic crystals, crystal engineering

MS.29.1

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X-ray crystallography and HIV vaccine design

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The human immunodeficiency virus (HIV) has evolved to evade host immune responses. Even after years of infection and elicitation of high levels of HIV-specific antibodies, most HIV infected individuals have ineffective antibodies, which do not neutralize circulating strains of primary HIV. Because HIV is an enveloped virus, the only viral proteins available to neutralizing antibody reside on the viral spike, which is composed of three copies of the exterior gp120 envelope glycoprotein and three copies of its gp41 transmembrane partner. While the viral spike has resisted atomic-level structure analysis, crystallographic structures of gp120 reveal dense carpets of glycan, evidence for epitope-masking conformational change, and hypervariable surface loops, all of which confirm the challenge of eliciting neutralizing antibody. Despite these difficulties, a few broadly neutralizing antibodies have been identified. We have characterized the structures for two of these antibodies, 2F5 and b12, in complex with their target epitopes. It has been suggested that immunization with precise mimics of these target epitopes might focus the immune response to appropriate sites of vulnerability. X-ray crystallography can assist at each step in the design process, by providing atomic-level mechanisms of evasion, atomic-level descriptions of sites of vulnerability, and structure-based techniques of immunogen design. Progress with each these steps will be presented, with a focus on structure-based immunogen design involving epitope transplantation into both heterologous and homologous scaffolds.

Keywords: immune system, virus host interaction, antibody

MS.29.2

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What we can learn from the structure of viral RNA-dependent RNA polymerases

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RNA dependent RNA polymerases (RdRPs) are the catalytic components of the RNA replication and the central players in the life cycle of RNA viruses. RdRPs are also a major target for the development of antiviral compounds. RNA viruses are exceptionally diverse in replication strategies, genetic organization, morphology and many other characteristics. Such differences raise significant questions about the diversity of virus origins and the possible extend of functional and evolutionary relationships among existing viruses. These issues are important not only for increasing our basic biological understanding but also for practical applications, since underlying similarities linking virus classes could provide a basis for antiviral approaches that have a broader spectrum. Our recent structural study of a Birnavirus RdRP reveals structural and functional links between positive-strand and double-stranded RNA viruses. We will summarize here the structural and biochemical studies of two different classes of viral RdRPs:
i) The polymerase 3D of foot-and-mouth disease virus, a member of the Picornaviridae family that possesses a linear plus strand RNA genome.
ii) The polymerase VP1 of infectious bursal disease virus, a member of the Birnaviridae family with double stranded RNA bipartite genome.
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Keywords: RNA-dependent RNA polymerase, RNA viruses, viral protein