

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

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Crystal structure of 6PicTubenzo thiourea derivative, oxidative cyclization and coordinated with Cu²⁺

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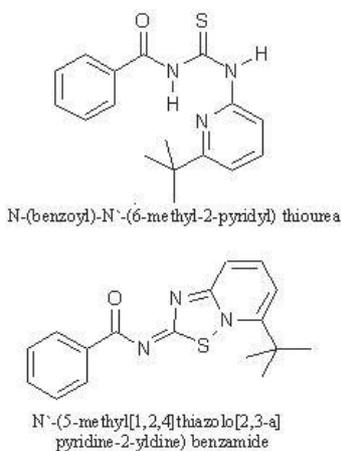
Thiocyanates (sulphocyanate or thiocyanide) are analogous to the cyanate ions. The reaction of these compounds with amine groups in the different materials form ourea and thiourea derivatives. The complexes of thiourea and thiourea derivatives are important since they have shown antitumor, antiviral, 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 isothiocyanate and 6-methyl-2-pyridyl. Then, (6picTu(Benzo)) reacts with the CuCl₂ in ethanol solution. The oxidative cyclization occurs and is generated N'-(5-methyl[1,2,4]thiazolo[2,3-a]pyridine-2-ylidene)benzamide. The new complex is build by this product and CuCl₂. CHN, AA-, IR-, ¹HNMR- and ¹³CNMR spectroscopies are used to characterize the products.

The crystal structures of these compounds from suitable solvents are determined with X-ray single crystal diffraction.

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Keywords: benzoyl isothiocyanate, benzoyl thiourea,

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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(salicylideneiminato)dibutyltin(IV) dichloride crystallises in monoclinic, C2/c space group with the unit cell parameter, $a = 15.0080 \text{ \AA}$, $b = 14.0472 \text{ \AA}$, $c = 14.2802 \text{ \AA}$ and $\beta = 112.703^\circ$. 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(salicylideneiminato) ligand forming a polymeric chain. On the hand, N-(2-Amino cyclohexyl)(salicylaldiminato)dichlorophenyltin(IV) chloroform solvate, crystallizes in monoclinic, P2₁/n with the unit cell parameter, $a = 11.559 \text{ \AA}$, $b = 11.877 \text{ \AA}$, $c = 18.766 \text{ \AA}$ and $\beta = 108.449^\circ$. 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(salicylideneiminato) 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-phenylenebis(salicylideneaminato)dicyclohexyl(IV) which crystallises in monoclinic, P2₁/c space group with the unit cell parameter, $a = 10.1419 \text{ \AA}$, $b = 17.2985 \text{ \AA}$, $c = 16.990 \text{ \AA}$ and $\beta = 102.668^\circ$. 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

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Unusual C-Br... π 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...C γ distances of 3.846(2) and 3.5983(12) \AA and C-Br...C γ angles, 168.42(9) and 171.66(8) $^\circ$ respectively, where C γ represents the centroids of unsubstituted cyclopentadiene rings of the ferrocene molecules.