

## Poster Sessions

molecule. Each 2,2'-iminobenzoate unit is linking two Cu(II) ions in a bis-bidentate mode, and the phenantroline unit is acting as a blocking ligand. The unit cell parameters are:  $a = 31.7600(5)$ ,  $b = 9.8517(2)$ ,  $c = 14.4899(3)$  Å,  $\alpha = 90$ ,  $\beta = 113.204(1)$ ,  $\gamma = 90^\circ$ ,  $V = 4167.00(14)$  Å<sup>3</sup>, space group C 2/c.

The magnetic properties of both compounds, namely the magnetization in function of the applied magnetic field and the susceptibility in function of the temperature will be presented and discussed.

**Keywords:** coordination compound, molecular magnetism, Cu(II) chain

### MS66.P19

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#### Effect of low Sr-Ba on the transport and magnetic behaviour of $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$

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The optimally doped composition ( $x=0.33$ ) of the intermediate bandwidth manganite system  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  has been studied extensively since the observation of large negative magneto resistance and strong ferromagnetism [Jin.S et al 1994]. In this compound, the double-exchange mechanism (DE) and electron-lattice coupling are believed to play major role in the occurrence of phenomena such as Ferromagnetism (FM), insulator-metal transition and colossal magneto resistance [Millis.A.J et al1995]. It is known that the substitution of cations of different size for A-site ions ( $\text{La}^{3+}$  and  $\text{Ca}^{2+}$ ) affects the unit cell structure and the corresponding changes in the distortion or rotation of  $\text{MnO}_6$  octahedrons give rise to wide variety of electronic properties [Hwang.H.Y et al 1995]. The conduction bandwidth of  $e_g$  electrons of Mn ions for instance is known to be strongly affected by the average size of A-site cations. By increasing the value of the latter by substitution method, both the conductivity and the paramagnetic to ferromagnetic transition temperature ( $T_C$ ) may be increased. In this context the electronic transport and the magnetic susceptibility properties of optimally doped compounds  $\text{La}_{0.67}\text{Ca}_{0.25}\text{Sr}_{0.04}\text{Ba}_{0.04}\text{MnO}_3$  (LCSBMO) and  $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$  (LCMO) synthesized under identical conditions are studied and compared. In the former composition, the average size of A-site ions has been increased lightly by simultaneous substitution of small percentage of large size ions such as  $\text{Sr}^{2+}$  and  $\text{Ba}^{2+}$  for  $\text{Ca}^{2+}$  ions. The focus of this work has been to study the effect of this low level substitution on the structural, microstructure, electronic transport and magnetic susceptibility properties of this widely studied LCMO. The electrical parameters which arise out of the fitting of standard models with resistivity data for  $T < T_{MI}$  and  $T > T_{MI}$  are compared and discussed in the above context apart from the paramagnetic to ferromagnetic transition temperatures ( $T_C$ )

**Keywords:** electronic transport, magnetic measurements,  $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$

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#### Classification of stacking interaction geometries of terpyridyl complexes

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Stacking interactions of terpyridyl square-planar complexes in crystal structures were studied analyzing data from the Cambridge Structural Database. In most of the crystal structures, two terpyridyl complexes were oriented “head-to-tail” or “head-to-head”, with “head-to-tail orientation” being most prevalent. The number of structures with other orientations was very small. Based on the analysis of interacting geometries, we classified overlaps of terpyridyl complexes into six types. The types were defined by values of several geometrical parameters and all interactions of the same type had very similar overlap patterns. Stacking interactions of aromatic nitrogen-containing ligands were geometrically analyzed in crystal structures of metal complexes. The results show that nitrogen-containing aromatic rings usually form an offset (or parallel-displaced) stacking interactions. A terpyridine (2,2';6',2''-terpyridine) molecule coordinating to a metal ion forms a large planar system of five rings, three pyridine fragments and two chelate rings. This planar system has propensity to form stacking interactions. Stacking interactions between terpyridyl complexes were observed in crystal structures and in solution. Recent review papers present interesting properties of terpyridyl complexes from luminescence to biological activity. Propensity for stacking interactions is important for using these complexes in biochemistry, supramolecular and medicinal chemistry [1].

[1] G. Janjic, J. Andric, A. Kapor, Z.D. Bugarčić, S.D. Zarić, *CrystEngComm*, **2010**, *12*, 3773-3777.

**Keywords:** stacking, CSD, terpyridine

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#### Structural Studies of $\text{N}_4\text{O}_2$ Iron(II) Spin Crossover Complexes

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Spin crossover (SCO) materials are molecular compounds switchable between a diamagnetic low-spin state (LS), which is stable at low temperatures and a paramagnetic high-spin state (HS), which is stable at higher temperatures. In general, the switching process in solid-state systems is controlled by cooperative intermolecular interactions. The correlation of structure with physical properties is crucial to the identification of these interactions and ultimately the understanding of the complex processes that control the SCO phenomenon.

We have carried out the syntheses and crystal structure analyses of iron(II) complexes with  $\text{N}_4\text{O}_2$  coordination spheres using the tridentate Schiff base ligand, 4-hydroxy-N'-((pyridin-2-yl)-methylene)-benzohydrazide (HL) previously reported by Zhang *et al.* [1] In the mononuclear complex  $\text{FeL}_2$  the average bond lengths Fe-N and Fe-O are 0.25 and 0.14 Å shorter in the low-spin state compared with the high spin state. These variations allowed us to characterise the spin states of other  $\text{N}_4\text{O}_2$  iron(II) complexes under different environmental conditions.

We have synthesised the mononuclear complexes  $\text{FeL}_2$  in methanol, ethanol, isopropanol and butanol to obtain different solvates. The crystals obtained from these reactions exhibit different spin states at room temperature indicating the importance of the crystal packing for the SCO phenomena. The figure shows the differences between (a) the structure of  $\text{FeL}_2 \cdot \text{EtOH}$  (LS) and (b)  $\text{FeL}_2 \cdot 2\text{H}_2\text{O} \cdot \text{PrOH}$  (HS). We have