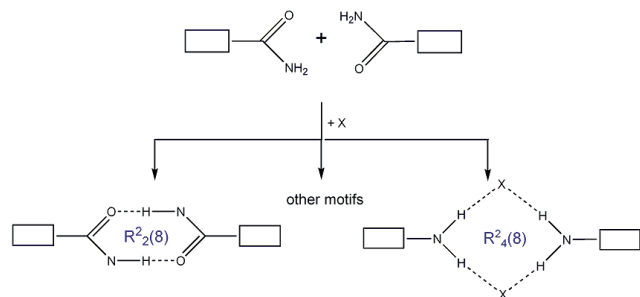


tetrameric motifs involving different accepting atoms, mostly halogens, are observed in seven of seventeen structures. Therefore, it would be of interest to determine the main factors influencing the outcome of supramolecular synthesis.

With this intention here we report a series of picolinamide complexes. The complexes have been characterized using single crystal X-ray diffraction, in addition to variety of thermal and spectroscopic techniques.



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Keywords: hydrogen bonding, amide supramolecular synthons, crystal engineering

MS17.P14

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The role of metal ion choice on the structure of coordination polymer materials

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The ability to predict the nature of intermolecular forces and manipulate these in the design of property specific supramolecular entities is still a significant scientific challenge today. This quest for the design of novel functional materials has led to active study in areas such as crystal engineering and supramolecular chemistry. One of the most studied areas at the moment is the creation of novel metal-organic frameworks or coordination polymers due to the possibility of using metal ions to align molecules in desired directions. However, complexes composed of first-row transition metals and monocarboxylic acids acting as both linkers and ligands are relatively rare and as a consequence there is an interest to develop methods for the synthesis of such complexes and to study their properties [1]. One of the envisaged uses of such materials is as single-chain and single-molecule magnets.

In this work the effect of the coordination characteristics of divalent Zn, Co and Mn on structures involving monocarboxylic acids has been examined. Several 1D and 2D coordination polymers have been synthesized and their structures determined. Typical 1D structures are composed of chains in which divalent metal ions (Zn^{2+} , Co^{2+} or Mn^{2+} for example) form a polymeric chain surrounded by carboxylate ligands. In all cases the carboxylate ligands coordinate to two metal ions and as a consequence act as a bridge between them, with the coordination environment being either tetrahedral (T_d) or octahedral (O_h) in some structures, or a combination of both in others. In these structures, Zn has a tendency to form complexes with either T_d or O_h coordination geometry, while Co prefers to form O_h but is also able to form T_d and other coordination geometries in between. This flexibility

in coordination usually results in 1D chains when Co or Zn are used. Mn^{2+} on the other hand, almost exclusively forms coordination sites with O_h geometry and as a consequence forms a more diverse array of structures to satisfy this requirement. This variety of coordination amongst these metals leads to a variety of structures - varying from cluster molecules to 1D chains and 2D nets - depending on the metal ion.

In addition, subtle alteration of organic ligand can significantly alter the coordination environment, and hence the structure of a material, offering further opportunities for structure manipulation. Other workers in this field have shown that in a 1D magnetic material that even very small changes in the weak interactions between the coordination polymer chains can significantly affect the properties of the material [1]. As a consequence, the effect of the systematic alteration of the organic ligands and metal ions on the crystal structures of several materials has been examined and will be presented.

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Keywords: crystal engineering, coordination polymer, crystal structure

MS17.P15

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Effect of ligand functionality in the structure of Zn^{II} 1D coordination polymers

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Although Zn^{II} metal-organic framework's are within the first examples of this kind of compounds to be prepared,¹ the interest in frameworks containing Zinc is still high due their interesting properties and potential applications.² Because of its spherical d^{10} configuration the Zn^{II} ion has a flexible coordination environment than can lead to zinc complexes with variable dimensionality.³ Hence an appropriate synthetic strategy can result in new Zn MOF's with 1D, 2D or 3D dimensionalities

One of our research areas is focused on the synthesis of MOF containing $Zn(II)$. In this contribution we report the synthesis and structural description of three 1D Zn^{II} coordination polymers using as organic linkers amino-carboxylate ligands derived from functionalized benzoic acid.

The reaction of the appropriate $Zn(II)$ precursors ($Zn(NO_3)_2 \cdot 6H_2O$ or $Zn(CH_3COO)_2 \cdot 2H_2O$) with 4-aminobenzoic acid (4-abaH), 4-(methyl)aminobenzoic acid (4-mabaH) and 3,4-diaminobenzoic acid (3,4-dabaH) generates the species $\{[Zn(4-aba)_2(H_2O)] \cdot (H_2O)\}_n$ [1], $\{[Zn_2(\mu-4-maba)_3] (\mu-4-maba)\}_n$ [2], and $\{[Zn(3,4-daba)_2(H_2O)_2] \cdot (H_2O)\}_n$ [3].

These three compounds show a 1D structure 1D where the metal centres are linked by amino-carboxylate ligands. Both **1** and **3** consist of one-dimensional chains in which the metals have similar environments. Two of the ligands are bonded by the amino group and the other two by the carboxylate group. However the presence of a methyl group in the amino moiety of 4-(methyl)aminobenzoic

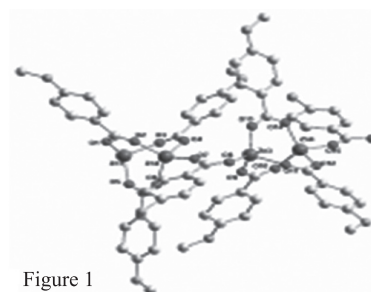


Figure 1