= 5.4456(3), *b* = 10.0655(5), *c* = 12.2423(8) Å, *β* = 96.997(6) and *Z* = 2. The molecular structure shows also helix type propagation along *b* axis. The helical structure is supported by H bonds involving N and Cl, forming an infinite zig-zag chain along *ab* plane.
Relevant structural parameters are the C=O and CO-C bond lengths on the ester group. They are somewhat shorter than those previously reported for the ethyl esters of some *S*-alanine and glycine derivatives, whereas the O2-C2 bond (the C-O bond of the butoxy group) is almost the same as the one of the mentioned derivatives [2, 3, 4, 5, 6].

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Keywords: Alaninate, Electron Density Topology, Helix propagation.

FA4-MS33-P15

Conformation effect in engineering a new magnetic materials. Amel Messai [a], Amani Direm [a], Nourredine Benali-Cherif[a], Dominique Luneau [b], [a]*Laboratoire des Structures, Propriétés et Interactions Inter Atomique (LASPI2A).Centre Universitaire de Khenchela 40000-Khenchela, Algérie.* [b]*Laboratoire de Mutlimatériaux et Interfaces (UMR 5615) Université Claude Bernard Lyon 1, Campus de la Doua 69622 Villeurbanne cedex, France*
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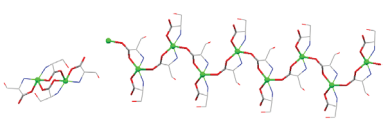
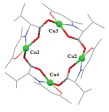
Among all the potentialities of coordination chemistry, molecular magnetism is very promising as magnetic information can be stored on one molecule. In that sense we developed in our group several strategies in order to obtain such molecular magnets. The idea was to use Schiff base ligands and cupper to generate high nuclear complexes.
Complexation of different conformation Shiff bases with copper (II) has been investigated. Tetranuclear complex with a cubane like core have been synthesised with conformation DL (Sciff base). With the same base D conformation we obtain a single magnetic chain



Chain of CuL



Cu_4 L_4

In this poster, we report the effect of the conformation of the ligand to obtain a different structure and properties, also we report synthesis, crystal structure and magnetic properties of the tetranuclear compound (Cu_4 L_4), and a single chain of copper (CuL)

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Keywords: Cluster-assembled materials, magnetic compounds, absolute configuration.

FA4-MS33-P16

Structural and conformational analysis studies of a 3*x*3 isomer grid of Methyl-*N*-(pyridyl)benzamides. Pavle Mocilac[a], Alan J. Lough[b], John F. Gallagher[a]
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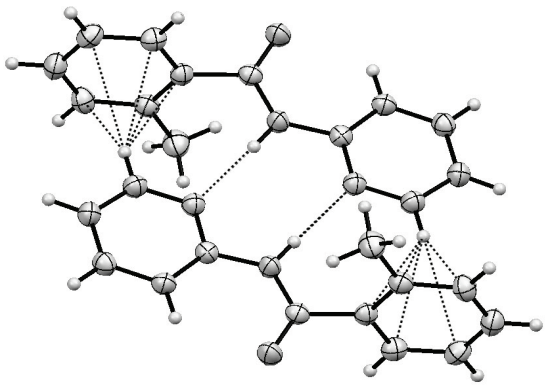
A 3*x*3 isomer grid of nine Methyl-*N*-(pyridyl)benzamides ($C_{13}H_{12}N_2O$) as **Mxx** (**x** = *para*-/*meta*-/*ortho*-) was examined to evaluate structural relationships from both *ab initio* calculations (*gas-phase*, PCM-SMD solvation model) and the solid-state. The effect of methyl group (**Mx**) and pyridine N atom (**x**) substitution patterns on molecular conformations from calculations and in terms of molecular organization is evaluated. Eight isomers form N-H…N hydrogen bonds with only **Mpm** having N-H…O=C interactions. The N-H…N interactions form *C*(6) chains in the **Mxp** series, *C*(5) chains in **Mmm**, **Mom** and cyclic centrosymmetric rings in the **Mxo** series. In **Moo** (below) a short *intra*-dimer C-H…π(arene) interaction is observed.



The solid state structures and conformations from calculations are mismatched in four **Mxx** molecules, in which the solid state structures adopt *meta*-stable or unstable conformations relative to the optimized computational models. The solvation model has no effect on the conformational trends, but decreases the rotational barriers making a conformational transition more probable, especially in more polar solvents.

Keywords: benzamides, conformational analysis, *ab initio*