A supramolecular approach to the analysis of the crystal structures of some 1-Alkyl-3-methyl-4-acyl-5-pyrazolone derivatives

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For theoretical and practical reason pyrazolones are an important group of nitrogen heterocyclic organic compounds. They find applications as analgesic and anti-inflammatory drugs, dyes, chelating extractants for numerous metal ions[1]. Pyrazolones have also attracted much attention because they exhibit prototropic tautomerism and they have been extensively studied both in solution and in the crystalline phase. Pyrazolones have also been studied as photochromic and luminescent materials. Coordination chemistry of pyrazolones is also very important; consequently considerable effort has been devoted to have a better knowledge of both ligands and metal complexes based on pyrazolone derivatives.

Most 3-aryl-4-acyl-pyrazolones reported to date are 1-aryl derivatives, in some few cases it is possible to found 1-alkyl examples like methyl or t-butyl, but the 1-n-alkyl-pirazolones are scarce. On the other side, it was shown that 5-pyrazolone can be easily alkylated at N-1 with primary alky halides yields being very good [2]. Alkylpyrazolones underwent electrophilic substitution at C-4 the same way 1-arylpiprazolones do. Thus, 1-n-alkylpyrazolones can be acetylated following the procedure reported by Jensen [3]. The 1-aryl-4-acetylpyrazolones are isoelectronic with β-diketones and their coordination chemistry is very well known. The coordination chemistry and tautomeric behaviour of some 1-n-alkyl-4-acylpyrazolones is even less known. In this presentation the synthesis and crystallographic data of 1-alkyl-3-methyl-4-acyl-5-pyrazolones and their Cu(II) complexes are discussed.

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Amide to amide interactions: from strong to weak hydrogen bonds in bis-(quinoline-carboxamide) functionality

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Deliberate design of molecules to build supramolecules in crystals with particular properties has become a very attractive area of research. A productive strategy in crystal engineering is to consider the molecules with functional groups that form robust synths [1]. Crystal packing is the result of the optimization of various possible intermolecular interactions between the molecules. Structures including carboxylic