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Supramolecular chemistry of pyridine- and pyrazine-carboxylic acids with Cu (I)

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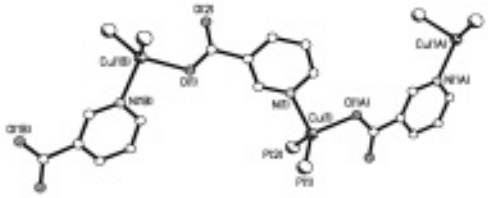
Keywords: supramolecular chemistry, hydrogen bonding, coordination polymers

We have been investigating the chemistry of pyridine and pyrazine carboxylates with the readily prepared starting material $[(PPh_3)_2Cu(BH_4)]$[1]. The $[BH_4]^-$ unit is readily displaced by the pyridine/pyrazine acids to yield coordination polymers or molecular species, depending on the acid and the solvent system used.
This poster will present recent results with pyridine and pyrazine carboxylic acids. In all cases the copper(I) centre adopts a tetrahedral geometry. The disposition of the pyridine/pyrazine and carboxylate groups is used to ''engineer'' desired polymeric architectures.



An example with pyridine-3-carboxylic acid is shown above which was the subject of an incomplete structural report in 1983[2].

[1] Lippard, S. J..; Ucko, D. A. *Inorg. Chem.,.* 1968, 7, 1051.
[2] Cariati F.; Naldini L.; Panzanelli A.; Demartin F.; Manassero M. *Mat. Inor. Chim. Acta*, 1983, 69, 117.

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Structural Study of a Designed Series of Compounds Featuring Rigid Molecular Geometry and Specific Fluorine Substitution

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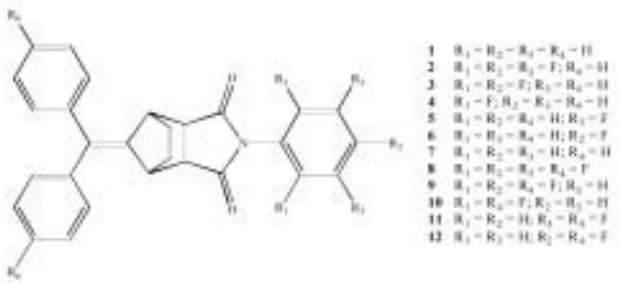
Supramolecular interactions including C-F•••H, F•••F, C-F•••π and aryl-perfluoroaryl contacts formed in crystalline solids of organic fluorine compounds have attracted considerable interest in the recent years due to their potential in crystal-engineering and materials design.[1] This has stimulated the synthesis and structural study of particular fluorine containing molecules and supramolecular constructions.[2, 3] Nevertheless, there are many open questions.
In order to go more deeply into the problem, compounds that feature not only a defined molecular geometry but will also allow easy modification of fluorine substitution would be a helpful test. This has given rise to a designed series of compounds **1-12**, the crystal structures of which are discussed here, laying particular stress on fluorine affected contacts and modes of supramolecular interactions competing with the interactions emanating from the presence of the O and N atoms.



[1] K. Reichenbächer, H. I. Süss, J. Hulliger, Chem. Soc. Rev., 2005, 22-30 and references therein.
[2] A. Schwarzer, W. Seichter, E. Weber, H. Stoeckli-Evans, M. Losada, J. Hulliger, CrystEngComm 2004, 6, 567-572.
[3] K. Reichenbaecher, H. Stoeckli-Evans, E. Weber, J. Hulliger, J. Fluorine Chem. 2006, 127, 270-276.