structure (Fig. 1), which is concentrated on the determination of the positions of hydrogen atoms.

In this compound the layered structure consists of infinite squared networks of \([\text{Co(HCOO)}_2]\). Urea molecules are sandwiched between neighboring layers acting as their supports. No direct covalent bond seems to exist between the layers of \([\text{Co(HCOO)}_2]\), except hydrogen bonds. This would prohibit a three-dimensional exchange interaction. Two dimensionality of exchange interactions in a three-dimensional framework is practically actualized in the present crystal. Especially this monoclinic crystal indicates weak-ferromagnetism. In this structure, an asymmetric unit contains two geometrically different molecules, where a Co ion is surrounded by other Co ions of different sites in the a-b plane. Therefore the uncancelled weak-ferromagnetic moment remains even if Co ions are coupled antiferromagnetically.

We determined the positions of 20 hydrogen atoms in this crystal, by difference Fourier synthesis and least squares refinement. And we have found some different types of the hydrogen bonds in it (Fig. 2). We will discuss the role of the hydrogen bonds in this crystal based on the accurate positions of hydrogen atoms.

![Fig. 1](image1)  
Fig. 1  
the monoclinic structure of CoFoul

![Fig. 2](image2)  
Fig. 2  
Hydrogen bonds between the layers structures

**TYPE OF HYDROGEN BOND**

(1) urea pair, (2) reconnect, (3) interlayer, (4) interlayer

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**PS-07.05.04**  
THE TRIFLUOROACETATE (AND TRIFLUOROACETATE) GROUP, CF\(_3\)COO- (TFA).  
By J.T. Ghosh and R.W. Small, School of Physics and Materials, The University, Lancaster, UK.

Using data from the Cambridge Structural Database, 414 separate determinations of the structure of the TFA group are reviewed. 194 published crystal structure determinations were involved. A comparison of the resulting molecular parameters is made with those obtained from theoretical calculations for the trifluoroacetate ion and trifluoroacetic acid using a basis set at the 6-31G* level. The TFA group was studied because of the wide variations in the repulsive molecular parameters, in particular the torsion angles of the CF\(_3\) group relative to the ester bond. A planar structure is shown to be the distribution of the C-F, C-C and C-O distances and the angles involving the C-F bond over the 4 \(\Phi\) structures grouped according to whether the group is mono or biesterate (170, 244, respectively). Mean parameter values and standard deviations of the group were 1.292(57) \(\AA\) (all structures), 1.530(41) \(\AA\) (all structures), 1.342(55) \(\AA\) (biesterate structures), 1.301(38) \(\AA\) (monoesterate structures), C-O = 1.250(37) \(\AA\) (monoesterate structures). The torsion angle involving CF\(_3\) for both mono and biesterate groups are spread over all possible values, consistent with rotational CF\(_3\) disorder. Consequently, the uncertainty of the position of the F atoms is at least \(\pm\) 1 \(\AA\) in the atomic displacement than radially. In the theoretical study the following molecular parameters were obtained - in the TFA anion \(\angle\) C-F = 1.365 \(\AA\), C-C = 1.559 \(\AA\), C-O = 1.294 \(\AA\), barrier to rotation of C-F 0.07 kJ/mol. For trifluoroacetic acid \(\angle\) C-F = 1.346 \(\AA\), C-C = 1.378 \(\AA\), C-O = 1.213 \(\AA\), C-O = 1.328 \(\AA\), barrier to rotation of C-F 0.61 kJ/mol.

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**PS-07.05.05**  
A COMPARISON OF THE CHEMISTRY OF CARBOXYLIC ACIDS OF PYRAZINE AND THEIR ESTERS  
WITH CuCl\(_2\).  
By Y. Wang and H. Stoeckli-Evans, Institute of Chemistry, University of Neuchâtel, Avenue de Bellevaux 51, CH-2000 Neuchâtel, Switzerland.

The ligand 2,5-dicarboxylic acid-5,6-dimethyl-pyrazine on reaction with CuCl\(_2\) at room temperature gave a green precipitate which was insoluble in water and organic solvents. Physical and chemical analyses indicate it to be a polymer. The reaction of the dimethyl ester gave a mononuclear complex (1) where one ester group has been hydrolysed to the acid which has then coordinated to the copper atom.

The reaction of pyrazine-2,3-dicarboxylic acid with CuCl\(_2\) also gives a pale green precipitate, the structure of which is thought to be a polymer (Antinelli & Pàris, 1972). The same reaction with the di-ester gave a pale green-blue solid. Physical and chemical analyses lead us to believe that it is a mononuclear complex. We will report on our latest results concerning the reaction of pyrazine and pyridine esters with Cu(II) and other 3d metals.  

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**PS-07.05.06**  
A DIOXANOCINIC COMPOUND WITH AN OXYGEN COORDINATED TRIGONAL PLANAR ZINC ATOM.  
By G. Bülow, H.-J. Gaiss* and G. Raabe, Institut für Organische Chemie, RWTH Aachen, Prof.-Pirlet-Straße 1, D-52056 Aachen, Germany.

Bis[(dimethylisopropoxysilyl)methyl]zinc (C\(_2\)H\(_5\)ZnSi\(_2\)O\(_3\)) crystallizes in orthorhombic space group P2\(_1\)2\(_1\)2\(_1\) with \(a=8.071(3)\) Å.