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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 $[Co(HCOO)_2]_4$. Urea molecules are sandwitched between neighboring layers acting as their supporters. No direct covalent bond seems to exist between the layers of $[Co(HCOO)_2]_4$ 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.

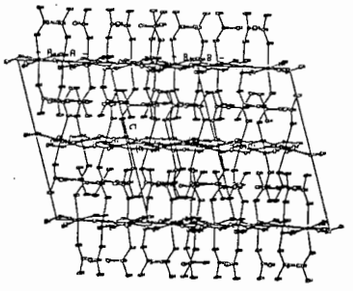


Fig. 1 the monoclinic structure of CoFoUr

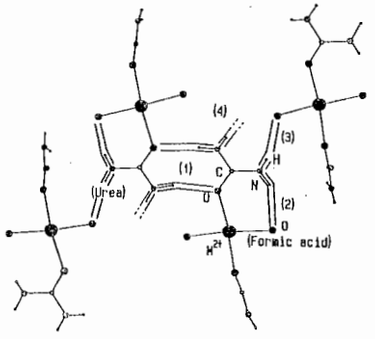


Fig. 2 Hydrogen bonds between the layers structures
TYPE of HYDROGEN BOND
(1) urea pair, (2) reconnect, (3) interlayer, (4) interlayer

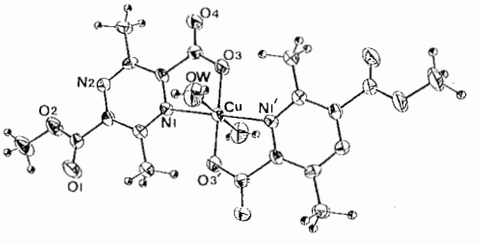
PS–07.05.04 THE TRIFLUOROACETATO (AND TRIFLUOROACETATE) GROUP, CF3COO- (TFA). By J.T. Gleghorn and R.W.H. Small*, School of Physics and Materials, The University, Lancaster, UK.

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 reported molecular parameters, in particular the torsion angles of the CF3 group relative to the carboxyl. Detailed plots will be shown of the distributions of the C-F, C-C and C-O distances and the angles involving the C-F bonds over the 414 structures grouped according to whether the group is mono or bidentate (173, 241 respectively). Mean parameter values and esd from the distributions of the reviewed structures are:-

C-F = 1.292(57) Å (all structures), C-C = 1.530(41) Å (all structures), projected F-C-F angle = 120° (assumed) esd 8.8° (all structures), C-O = 1.242(53) Å (bidentate structures), C=O = 1.213(38) Å (monodentate structures, C-O- = 1.250(37) Å (monodentate structures). The torsion angles involving CF3 for both mono and bidentate groups are spread over all possible values, consistent with rotational CF3 disorder. Consequently, the uncertainty of position of the F atoms is at least 3 times greater in the azimuthal direction than radially. In the theoretical study the following molecular parameters were obtained:- in the TFA anion, C-F = 1.365 Å, C-C = 1.559 Å, C-O = 1.254 Å, barrier to rotation of CF3 0.07 kcal/mol. For trifluoroacetic acid C-F = 1.346 Å, C-C = 1.538 Å, C=O = 1.213 Å, C-O- = 1.342 Å, barrier to rotation of CF3 0.61 kcal/mol.

PS–07.05.05 A COMPARISON OF THE CHEMISTRY OF CARBOXYLIC ACIDS OF PYRAZINE AND THEIR ESTERS WITH $CuCl_2$. By Yi Wang* and H. Stoeckli-Evans, Institut de Chimie, Université de Neuchâtel, Avenue de Bellevaux 51, CH-2000 Neuchâtel, Switzerland.

The ligand 2,5-dicarboxylicacid-3,6-dimethyl-pyrazine on reaction with $CuCl_2$ at room temperature gave a green precipitate which was insoluble in water and organic sovents. 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 the pyrazine-2,3-dicarboxylicacid with $CuCl_2$ at r.t. also gives a pale green precipitate, the structure of which is thought to be a polymer (Antinelli & Pâris, 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 3^d metals. J.-P. Antinelli & M.R. Pâris, C.R. Acad. Sc., Paris, 274,C51(1972).

PS–07.05.06 A DIORGANOZINC COMPOUND WITH AN OXYGEN COORDINATED TRIGONAL PLANAR ZINC ATOM. By G.Bülow, H.-J-Gais*, and G.Raabe*, Institut für Organische Chemie, RWTH Aachen, Prof.-Pirlet-Straße 1, D-5100 Aachen, Germany.

Bis[(dimethylisopropoxysilyl)methyl]zinc ($C_{12}H_{30}O_2Si_2Zn$) crystallizes in orthorhombic space group $P2_12_12_1$ with a=8.071(2),

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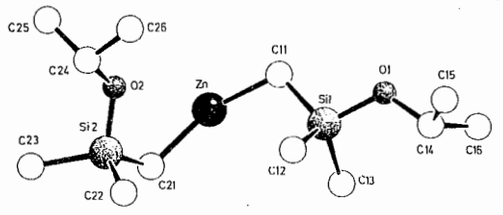
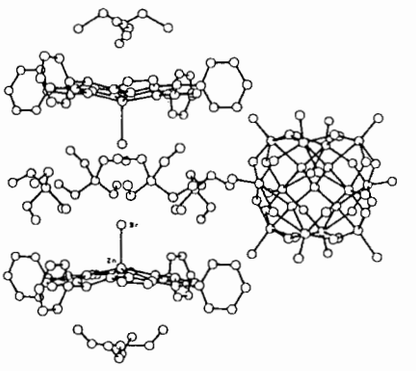
b=11.672(2), c=20.342(1)Å. $R(R_w)$=0.054(0.055), 2737 observed reflections, 135 refined parameters, MoK_α radiation, D_{cal}=1.137g·cm^{-1}, F(000)=704 (G.Bülow, H.-J.Gais, G.Raabe, 1993, *Organometallics*, submitted). In addition to two covalently bonded C atoms Zn is coordinated by an oxygen atom of a neighbouring molecule .As a result of this complexation the C-Zn-C moiety is significantly bent (152.3(3)°) and the molecules are arranged in helices perpendicular to the *bc* plane. The metal atom lies in a chiral plane and is in contact with another oxygen atom belonging to one of its covalently bonded ligands. The influence of complexation on the geometry of the C-Zn-C segment is substantiated by quantum chemical *ab initio* and semiempirical calculations. In addition the computational results indicate that the energy of complexation is rather low (≈-3 kcal/mol).



PS-07.05.07 A NEW TERNARY POLYOXOMETALATE CHARGE-TRANSFER SALT. By D. Attanasio[a], F. Bachechi[b]* and L. Suber[b], [a]Istituto di Chimica dei Materiali, [b]Istituto di Strutturistica Chimica, Area della Ricerca di Roma, C.N.R., C.P. 10, 00016 Monterotondo Staz., Roma, Italy.

Recently, a type of organic-inorganic charge-transfer compounds has received considerable attention. These materials consist of polyoxoanions as electron acceptors and a variety of organic molecules as donors.
As part of a study concerning polyoxoanions of the early transition metals in the α-Keggin structure and alkyl amines as organic donors, several ternary CT salts were synthesized and the crystal structure of one of them, $[(C_2H_5)_4N]_5$ $[(ZnTPP)_2SiMo_{12}O_{40}Cl]$, with ZnTPP = tetraphenylporphyrinatozinc(II), was determined.
These compounds contain two photoactive molecular entities, the metallo macrocycles and the α-Kegging units, which can give rise to electron transfer processes. This unexpectedly stable molecular association is made possible by the presence of the halide ion as third component.
The structure (space group $I\bar{4}$) is built by $SiMo_{12}O_{40}$ units at the origin of the I lattice. The two ZnTPP are located on the four-fold axis and are related by an inversion centre. Also the Br atom, coordinated to the Zn, and one molecule of $[(C_2H_5)_4N]^+$ lie on the four-fold axis and are disordered on two centrosymmetric positions. The other molecules of $[(C_2H_5)_4N]^+$ appear forming a layer which interposes between the two ZnTPP.



PS-07.05.08 CRYSTAL AND MOLECULAR STRUCTURE OF $[Ir(H)_x(Cl)_3(P^iPr_3)_2]$, 1 (x=1 or 2): ANOTHER EXAMPLE OF Ir^{IV} PARAMAGNETIC HYDRIDE OR AN IRIDIUM(V) COMPLEX, TRANSIENT INTERMEDIATE OF $[Ir^{IV}(H)_2(Cl)_2(P^iPr_3)_2]$, 2 ? By D. Capitani P. Mura* (I.S.C. "G. Giacomello" - Area della Ricerca C.N.R. Monterotondo Stazione Roma - Italy), and D. Ajò (I.C.T.R. Area della Ricerca C.N.R. Padova - Italy).

We recently reported on the unusual paramagnetic behaviour of Ir^{IV} and Rh^{IV} dihydrido complexes (D. Ajò, D. Attanasio, S. Lucente, P. Mura, A.L. Segre, F. De Zuane, J. Mag. and Magnetic Materials, 1992, 104-107, 1997-1998). Till now we have not a definitive explanation why the synthesis of 2 (P. Mura, A.L. Segre, S. Sostero, Inorg. Chem., 1989, 28, 2853-2858) sometimes give rise to samples having different μ_{eff}, and the magnetic moment of recrystallized samples show always lower values (μ_{eff}<1 BM) than spin only for a d^5, Ir^{IV} species. Complex 1 probably may help us to clarify the problem. The crystal structure of 1 show a slightly distorted octahedral geometry with the two P^iPr_3 phosphines in trans position as well as two chlorine atoms; the third Cl is in trans to the hydride(s) ligand(s).

Crystal data for 1.
Cryst. Syst. Triclinic, space group P1.

a=8.761(2)Å b=8.823(1)Å c=9.808(2)Å
α=100.66°(1) ß=91.20°(1) γ=119.72°(1)
V=641.39Å^3 F(000)=309.00 μ=5.64mm^{-1}
R=0.0588 wR=0.0706 for 2993 data (Fo>8σ(Fo))