09.4-27 CRYSTAL DATA AND COORDINATION NUMBER FOR SOME COMPOUNDS. By Tian-Huey Lu, Cheu-Pyeng Cheng and Chung-Sun Chung, National Tsing Hua University, Hsinchu, Taiwan 30043, China.

The three compounds now under investigation are: (1) (5, 7, 7, 12, 12, 14-hexamethyl-1, 4, 8, 11-tetraaza-cyclotetradeca-4, 14-diene) Copper(II) Perchlorate $Cu(C_{16}H_{32}N_4)(ClO_4)_2$; (2) (N-Carbamoylmethyl-trimethylenediamine) Copper(II) Perchlorate, $[Cu(H_2O)(C_5H_{13}N_3O)](ClO_4)_2$ and (3) 3,3'-dibromophenanthro-quinone-triphenyl-phosphinetricarbonyl-rhenium(O), $C_{35}H_{21}Br_2O_5PRe$. Their corresponding crystal system, space group and cell dimensions obtained from film picture taken by precession camera are: (1) Monoclinic, $P2_1/c$; a=9.99, b=10.3, c=10.6 Å, β=110°; (2) Orthorhombic, $P222_1$, a=6.77, b=11.2, c=13.6 Å, and (3) Tetragonal, $P4_22_12$, a=b=11.0, c=37.4 Å. Crystal data determined by counter and diffraction intensities collected by autodiffractometer will be processed as soon as the autodiffractometer is fixed. Consequently, three-dimensional crystal structure of these three compounds will be solved shortly.
Some metal(II) complexes whose structure has been solved are: (1) $[Cu(C_{16}H_{32}N_4)](ClO_4)_2$ [Acta Cryst. (1984). C40, 70-72]; (2) $[Ni(C_{20}H_{40}N_4)](ClO_4)_2.1.5H_2O$ [Proc. Natl. Sci. Coun. ROC (A), 8-4 (1984). 217-223]; (3) $[Cu(C_6H_{16}N_4O_2)(H_2O)].H_2O$ [Acta Cryst. (1984). C40, 1131-1135]; (4) $[Cu(H_2O)(C_{16}H_{36}N_4)](ClO_4)_2$ [Acta Cryst. (1986). C42, 801-803]; (5) $[Cu(C_{16}H_{36}N_4)(SCN)](ClO_4)$ [J.C.S. Dalton. in press]; (6) $[(Cu(C_{10}H_{22}N_4O_2)](ClO_4)](ClO_4)_3$ [accepted by Acta Cryst.]. and (7) $[Cu(NO_3)(C_8H_{18}N_4O_2)(H_2O)].NO_3.H_2O$ [Acta Cryst. (1984). C40, 1131-1135]. Their corresponding crystal system space group and cell dimensions are: (1) monoclinic, $P2_1/c$, a=10.331(5), b=10.641(5), c=11.050(6) Å, β=111.96(4)°; (2) tetragonal, $I\bar{4}$, a=b=25.89(2), c=8.598(8) Å; (3) monoclinic, $P2_1/c$, a=6.795(7), b=16.872(8), c=12.103(13) Å, β=118.02(8)°; (4) monoclinic, C2/c, a=11.993(1), b=13.057(2), c=15.969(4) Å, β=92.37(1)°; (5) monoclinic, $P2_1/n$, a=8.016(3), b=30.109(8), c=10.865(2) Å, β=104.93(2)°; (6) orthorhombic, Pnma, a=10.367(1), b=27.545(5), c=12.876(2) Å and (7) triclinic, $P\bar{1}$, a=7.663 (3), b=10.725(6), c=10.767(5) Å, α=91.82(4), β=108.18(9), γ=90.14(4)°. The corresponding coordinate numbers of the metal(II) are: (1) 4; (2) 4; (3) 5; (4) 5; (5) 5; (6) 5 and (7) 6. The first compound has no water and the perchlorate ion situates at a long distance beyond the bonding with copper. Although there is water in the second complex, yet the water forms hydrogen bond with the ligand and separates a distance from copper. Most copper(II) compounds stay in the state of five coordination number. In addition to the coordination of radical, NO_3^-, with copper(II), water squeezes into the bonding and makes the seventh crystal form six coordinations.

09.4-28 SYNTHESIS AND PHYSICAL PROPERTIES OF COPPER (II) COORDINATION COMPOUNDS WITH MESOMORPHIC PROPERTIES

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The coordination compounds or organometallic species having mesomorphic properties constitute a new class of materials which can find practical applications. Going on with our studies on such compounds (M.Ghedini, N. Longeri and R.Bartolino, Mol. Cryst. Liq. Cryst., 84, 207 - 1982; M.Ghedini, S.Licoccia, S.Armentano and R. Bartolino, Mol. Cryst. Liq. Cryst., 108, 269 - 1984) we present here an investigation on the copper (II) coordination compounds whose general formula is $((C_n H_{2n+1})(C_m H_{2m+1})(C_{13} H_8 NO_2))_2$ Cu(II). In particular we have extensively characterized the complex $C_{58} H_{84} N_2 O_4 Cu$, corresponding to n = 4, and m = 12, by elemental analysis, infrared spectroscopy, optical microscopy, differential thermal analysis and x-ray diffraction.

Elemental alalyses.
Calc.: C% 74.35; H% 9.03; N% 2.99. Found: C% 74.40; H% 9.05; N% 2.86.

Thermal behaviour (°C), textures and x-ray diffraction.

Solid 1 —81— Solid 2 —117— S_A —141— I

In particular x-ray analyses show an unusual diffuse peak in the pattern of the solid 2. Moreover the data suggest an interdigitation in the S_A mesophase.