

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 $\text{Cu}(\text{C}_{16}\text{H}_{32}\text{N}_4)(\text{ClO}_4)_2$; (2) (N-Carbamoylmethyl-trimethylenediamine) Copper(II) Perchlorate, $[\text{Cu}(\text{H}_2\text{O})(\text{C}_5\text{H}_{13}\text{N}_3\text{O})](\text{ClO}_4)_2$ and (3) 3,3'-dibromophenanthro-quinone-triphenyl-phosphinetricarbonyl-rhenium(O), $\text{C}_{35}\text{H}_{21}\text{Br}_2\text{O}_5\text{PRE}$. 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, $\beta=110^\circ$; (2) Orthorhombic, $P22_2$, $a=6.77$, $b=11.2$, $c=13.6$ Å, and (3) Tetragonal, $P4_22_2$, $a=b=11.0$, $c=37.4$ 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) $[\text{Cu}(\text{C}_{16}\text{H}_{32}\text{N}_4)](\text{ClO}_4)_2$ [Acta Cryst. (1984). C_{40} , 70-72]; (2) $[\text{Ni}(\text{C}_{20}\text{H}_{40}\text{N}_4)](\text{ClO}_4)_2 \cdot 1.5\text{H}_2\text{O}$ (Proc. Natl. Sci. Coun. ROC (A), 8-4 (1984). 217-223); (3) $[\text{Cu}(\text{C}_6\text{H}_{16}\text{N}_4\text{O}_2)(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$ [Acta Cryst. (1984). C_{40} , 1131-1135]; (4) $[\text{Cu}(\text{H}_2\text{O})(\text{C}_{16}\text{H}_{36}\text{N}_4)](\text{ClO}_4)_2$ [Acta Cryst. (1986). C_{42} , 801-803]; (5) $[\text{Cu}(\text{C}_{16}\text{H}_{36}\text{N}_4)(\text{SCN})](\text{ClO}_4)$ [J.C.S. Dalton. in press];

(6) $[\text{Cu}(\text{C}_{10}\text{H}_{22}\text{N}_4\text{O}_2)](\text{ClO}_4)](\text{ClO}_4)_3$ [accepted by Acta Cryst.]. and (7) $[\text{Cu}(\text{NO}_3)(\text{C}_8\text{H}_{18}\text{N}_4\text{O}_2)(\text{H}_2\text{O})] \cdot \text{NO}_3 \cdot \text{H}_2\text{O}$ [Acta Cryst. (1984). C_{40} , 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, $\beta=111.96(4)^\circ$; (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, $\beta=118.02(8)^\circ$; (4) monoclinic, $\text{C}2/c$, $a=11.993(1)$, $b=13.057(2)$, $c=15.969(4)$ Å, $\beta=92.37(1)^\circ$; (5) monoclinic, $P2_1/n$, $a=8.016(3)$, $b=30.109(8)$, $c=10.865(2)$ Å, $\beta=104.93(2)^\circ$; (6) orthorhombic, Pnma , $a=10.367(1)$, $b=27.545(5)$, $c=12.876(2)$ Å and (7) triclinic, $\text{P}\bar{1}$, $a=7.663(3)$, $b=10.725(6)$, $c=10.767(5)$ Å, $\alpha=91.82(4)$, $\beta=108.18(9)$, $\gamma=90.14(4)^\circ$. 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.Licocchia, 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 $((\text{C}_n\text{H}_{2n+1})(\text{C}_m\text{H}_{2m+1})(\text{C}_{13}\text{H}_8\text{NO}_2))_2\text{Cu}(\text{II})$. In particular we have extensively characterized the complex $\text{C}_{58}\text{H}_{84}\text{N}_2\text{O}_4\text{Cu}$, corresponding to $n=4$, and $m=12$, by elemental analysis, infrared spectroscopy, optical microscopy, differential thermal analysis and x-ray diffraction.

Elemental analyses.

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.