09.4-9 CRYSTALLINE AND MOLECULAR STRUCTURE OF (2-MERCAPTOBENZOXALATE) METHYLMERCURY(II) AND (2-MERCAPTO BENZOXALATE) PHENYLMERCURY(II). By Y.P. Mascarenhas, IFQSC/USP, C.P. 369, 13560, São Carlos, S.P., Brazil; K. Tomita, IQ-Araraquara, C.P. 174, 14800, Araraquara, S.P., Brazil; C.O.P. Santos, UNESP - Presidente Prudente, 19100, Presidente Prudente, S.P., Brazil; J.S. Casas, Dept. of Inorganic Chemistry, School of Pharmacy, U. of Santiago, Galicia, Spain.

The X-ray structure determinations were performed with the purpose of elucidate if the intramolecular secondary bond of Hg involved either the endocyclic nitrogen or oxygen. Furthermore, it is also of interest, to consider the role of these complexes in agricultural environments if we recall that the ligand itself is a fungicide, has bacteriostatic activity and is a regulator of plants growth. (Preti, C., Tosi, G. - J. Inorg. Nucl. Chem., 18, 1125 (1976)). Thus, it is quite possible that the organometalic contaminant of the environment and this ligand used in agriculture may naturally interact.

Crystal data for the phenyl Hg(II) complexes (A): $C_{13}H_9NoHg$, M.W. = 411,34, triclinic, $P\bar{1}$, a = 10.677(2), b = 11.176(6), c = 11.445(3) Å, α = 66.67(3), β = 86.55(2), γ = 78.69(3)°, V = 1229.4(9) Å^3, Z = 4, D_x = 2.22 g/cm^3, λ(MoKα) = 0.71073 Å, μ = 122 cm, F(000) = 792, T = ca 293°K, R = 0.075 for 2297 observed reflections (I > 3σ(I)), unit weights.

Crystal data for the methyl-Hg(II) complex (B): C_8H_7NOSHg, M.W. = 345.74, monoclinic, $P2_1$, a = 10.601(1), b = 8.164(3), c = 10.876(2)Å, β = 103.87(1), V= 913.83 Å^3, Z = 4, D = 2.51 g/cm^3, μ = 163.86, λ(MoKα) = 0.71073 Å, F(000) = 664, T = ca 293°K, R = 0.077, R_w = 0.076 for 1247 observed reflections (I > 3σ(I)), $w = (\sigma(F) + 0.003\,F)^{-1}$. Both structures were solved by Patterson and difference Fourier methods and refined by blocked L.S. method. An intramolecular secondary bond between Hg and the endociclic nitrogen was found for both complexes. For complex A the crystal packing may be described as discrete sets of dimerized molecules via Hg and S interactions between the two independent molecules present in assymetric unit with Hg-S'=3.33 Å and Hg'-S = 3.47. For complex B we have a much more complex network of intermolecular interactions involving Hg, S and O with Hg-S'(1) = 3.75 Å, Hg-O'(2) = 2.90 Å, Hg'-S(3) = 3.47 and Hg'-O(4)=2.86 Å where the primed and unprimed atom's names stand for the two independent molecules in the assymetric unit and the number in parenthesis for the following symmetry operations: (1) = x, 1.0-y, z; (2) = -x, 0.5+y, -z; (3) = x, 1.0+y, z; (4) = 1-x, 1.5+y, -z.

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09.4-10 CRYSTAL STRUCTURES OF SOME DITHIOCARBAMATES. By J. Garaj, V. Vrábel, E. Kellö and J. Lokaj, Dep. of Anal. Chem., Slovak Technical University, Bratislava, Czechoslovakia.

Several metal dithiocarbamate (dtc) compounds have been examined structurally in our laboratory. In the transition metal complexes all the sulphur-metal bond distances are almost equal, while there are two kinds of bond distances in the non-transition metal complexes.

The crystal structures of Na-salt of ethylenebis-dtc and $Bu_2Sn(pmdtc)_2$, $Bu_2Sn(morphdtc)_2$, $Bu_2Sn(Bu_2dtc)_2$ were solved by the heavy atom method and were refined by block diagonal least-squares. So far no information is available on crystal structures of ethylenebis-dtc complexes. The structure consists of infinite chains connected by 4 water molecules bridging both sides of organic anion. The geometry about Na-cations is distorted octahedral. In the Sn-dtc complexes the geometry about tin atoms is highly distorted from octahedral and cannot be considered as cis- or trans-octahedral. The anisobidentate coordination of each of the dtc ligands involves one short and one long Sn-S distance.

09.4-11 COMPLEXES OF CADMIUM HALIDES WITH 18-CROWN-6-ETHER. By A. C. Hazell, Chemical Institute, Aarhus University, DK-8000 Århus C, Denmark.

Macrocyclic ligands such as crown-ethers are of interest in that they force metal ions to have unusual coordination numbers and geometries, they have also been considered as models for studying the transport of metal ions across membranes.

The CdI_2 complex is orthorhombic, space group Pnma, a = 16.563(3), b = 27.996(5), c = 8.382(2) Å, Z = 8. There are two crystallographically independent molecules, one on a symmetry centre and the other on a mirror plane. Cadmium can be regarded as eight-coordinated with the complex having hexagonal bipyramidal geometry, or as two-coordinated with the linear CdI_2 groups "threaded" through the 18-crown-6 cavity. The mean Cd-I distance is 2.692(1) Å, Cd-O distances range from 2.69(1) to 2.81(2) Å with a mean of 2.768(4) Å.

The $CdBr_2$ complex is apparently rhombohedral, space group $R\bar{3}$, a = 7.879(3) Å, α = 96.88(3)°, Z = 1, and isomorphous with the $CdCl_2$ compound (Paige and Richardson, Can. J. Chem. 1984, 62, 332-335). However, solid state ^{113}Cd CP/MAS nmr spectra (Jakobsen, 1987) of the $CdCl_2$ and $CdBr_2$ complexes differ in that all the peaks in the spectrum of the bromide are split. The structure of the bromide is being determined to see if it really has a lower symmetry than that of the chloride or whether an explanation of the anomalous spectrum must be sought elsewhere.