STRUCTURES OF ORGANIC, ORGANOMETALLIC AND COORDINATION COMPOUNDS

09.4-10 COMPLEXES OF MACROCYCLIC POLYETHER DIAMIDES. By J. Hasek, J. Ondrček, and K. Huel. Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, 162 06 Praha, Czechoslovakia.

(I) Complex of 7,19-dibenzyl-2,2,3,3-tetramethyl-17,19-diaza-1,4,10,13,16-pentaoxacyclohexene-6,20-dione with strontium tetrachloro­phosphonate and nitromethane (2:1:2:2), monoclinic, P21/c, a=33.88(1), b=11.639(2), c=16.839(3) Å, \( b=120.23(2)^\circ \), \( B=2 \), (C\( _{32} \)H\( _{46} \)N\(_{2}\)O\(_{7}\)). Sr\( \text{2(C}_6\text{H}_5\text{Cl)}\text{4B.2CH}_3\text{N0}_2\). Crystals obtained by very slow evaporation have to be kept in a capillary. The refinement of non-H atoms revealed Sr... O at 2.503(6), 2.486(6), 2.758(5), 2.615(6) Å. Three etheric oxygens have no contact to Sr.

(II) The complex (I), where Sr was replaced by Ca, gave poorly defined crystals showing diffuse reflexions. Intensity statistics proposed space group P\( 2_1 / c \), a=14.68(2), b=17.28(2), c=23.97(5) Å, \( \alpha=80.1(1)^\circ \), \( \beta=83.0(1)^\circ \), \( \gamma=86.8(1)^\circ \), \( Z=2 \). The favourable effect of methyl substituents of the macrocycle in positions on the selectivity for calcium in PVC membranes, studied by Petrásček and Ryba (Anal. Chim. Acta, 1981, 128, 129)

09.4-12 THE CRYSTAL STRUCTURE OF S-CIS-DIAQUA [BIS(2-PYRIDYL)-3,6-DITHIAOCTANE 1 COBALT(III) DIPERCHLORATE. By A. Castellanos*, K. Hiltor*, M.V. Paladar*, J. Sordo* and J. Steidle**.

The crystal structure of the Co\( \text{C}_6\text{H}_{20}\text{N}_2\text{S}_2\)\( \text{(H}_2\text{O)}\)\(_{2}\) \( \text{(C}_4\text{O)}\)\(_{2}\) compound are monoclinic, space group P2\( 1 / n \), \( Z=4 \) with \( a=11.676(4) \) \( b=13.357(4) \), \( c=15.835(6) \) Å, \( \beta=107.33(3)^\circ \), \( V=2337.4 \) \( \AA^3 \), \( D_\lambda = 1.686 \text{ Mg m}^{-3} \). 7681 reflexions collected on a diffractometer using graphite monochromated MoK\( \alpha \). 3179 reflexions observed I > 3\( \sigma (I) \). The structure was refined to a final R value of 0.053.

The compound is built up from discrete Co\( \text{C}_6\text{H}_{20}\text{N}_2\text{S}_2\)\( \text{(H}_2\text{O)}\)\(_{2}\)\( \text{(C}_4\text{O)}\)\(_{2}\) and CO\( \text{ClO}_4 \) ions. In the distorted octahedral cations a single ligand molecule is coordinated to one Co via N and S atoms, forming one five-membered chelate ring (CoSC\(_2\)S) and two six-membered rings (CoSC\(_3\)N).

The two remaining coordination positions are occupied by water molecules. The perchlorate ions exhibit the expected tetrahedral geometry though somewhat deformed. They are H-bonded to \( \text{H}_2\text{O} \) coordinated molecules.

09.4-11 SYSTEMATICS OF METAL CYCLIDENE LACUNAR STRUCTURES. By W.M. Alcock, Department of Chemistry, University of Warwick, Coventry, CV4 7AL, England, and D. H. Busch, Department of Chemistry, Ohio State University, Columbus, Ohio 43210, U.S.A.

The transition metal complexes of the cyclidene unit (I) have as their key structural feature a void between the metal and the \( R^1 \) chain. Both the size of this void and its chemical nature can be adjusted by changing \( R^1 \), and chemical studies have shown that with appropriate metal ions (especially Fe(II), Co(II), Ni(II)), these complexes can (a) bind \( O_2 \) reversibly and (b) incorporate organic substrate molecules with the potentiality of carrying out chemical reactions within the cavity. Some 20 crystal structures of this group of compounds have now been determined, and these structural results will be analysed. They also include a precursor, in which \( R^1 \) is absent, which throws light on the ease of formation of the complexes, and dimers in which \( R^1 \) is a complete metal cyclidene macrocycle.