07-Crystallography of Organometallic and Coordination Compounds

Cu(II) with the carbon atoms of neighboring molecules. In Cu(acetilacetonate)$_2$, for instance, they are arranged in such a way that to form the chains along the shortest unit cell edge. Mixed-ligand complexes of Cu(II) are pseudooctahedral and the second form of Y(dipivaloylmethanate) is the dimeric one.

$\beta$-Diketonate complexes of alkaline-earth metals are oligomeric ones. Oligomerization extent depends on synthesis conditions. Complexes of the type II and III are "the guest-host complexed". The influence of the additional neutral ligands on oligomerization extent of complexes in condensed phase has been considered by those examples. The Cu complexes with crown ethers are chain polymers. Oxidantant binding of the donor atoms of the additional ligands by the metal atoms has been shown to result in monomeric complexes with high coordination numbers of metal atoms and normal Van-der-Waals interactions between the complexes. Conformation and symmetry changing of the additional ligands in complex formation of this type were considered.

The coordination polyhedron of metal atoms in volatile complexes and in the high-$T_c$ superconducting oxides were compared. It was revealed a lack of direct analogies between them in many cases.

Topological features of the central metal atoms arrangement in the complexes were treated. They have been shown to be represented by undeformed nets, having, for example, Schlafli symbols, $\{4,6\}_3$, and the shortest distances between metal atoms arranged in the nodes of the nets. A correlation between structures of the complexes and their volatility and thermostability has been discussed.

Introduction of additional ligands into guest-host complexes of type II and IIB has been shown to improve useful properties of compounds.

Fig. 1. Molecular structure of GD(ABA)·H$_2$O, a single chain, which intersects the double chain above at each Cd atom, presenting a two-dimension network structure. The Cd ion is 6-coordinate, bonded to six oxygen atoms from five carboxylate groups and to the three oxygen atoms of water molecules. There are two free water molecules in the unit cell. The Cd-O bond lengths range from 1.82 to 2.44 Å, one distance, namely, the Cd-O(21) of 2.41 Å, being significantly longer than the mean Cd-O bond length, 2.34 Å. The (210) atom is the upper vertex of the tetragonal pyramid. The (210) bridging bidentate) averaged distance of 2.35 Å is the longest, but the (2111) bridging bidentate) averaged one of 1.86 Å is the longest in the three coordination forms. The rest of Cd-O, unidentate, bridging part in tridentate) range from 2.17 to 2.35 Å (with S mean bond length of 2.2 Å). The bond lengths and angles of the ABA in this paper are about the same as those of the literature[Allen and Don, 1970].

References

PS-07.04.33 THE STRUCTURE OF CATIONIC COMPLEX WITH METHYLENE DICYANONITRILE (DMA). By Yan Xing, Keng-Cheng Jia, Zhi-Band Duan and Ji-Zuan Ni, Changsha Institute of Applied Chemistry Chinese Academy of Sciences, Changsha, People's Republic of China

Abstract GD(DMA)$_n$·$\cdot$H$_2$O, Mr, 229.4, triclinic, P1, a=24.14(4), b=14.19(3), c=21.98(4), $\alpha=92.1(1)$, $\beta=91.2(1)$, $\gamma=91.5(1)$, 7-1, R, 2, 2.44 g cm$^{-3}$. $\lambda$ (MoKa)=0.71069 Å, $\mu$=0.35 mm$^{-1}$ for 2634 observed reflections.

There are one and half ligands in an asymmetric unit. The molecular formula is GD(DMA)$_2$·H$_2$O. The molecular structure is shown in Fig. 1. The ligands are coordinated in two different forms in the molecule, (1) only one of the two carboxylic oxygen atoms is bonded to a metal ion, and the other one is free, secondly, two carboxylic oxygen atoms are coordinated to two different metal ions, forming a carboxylate bridge, preseing a double chain structure, thirdly, two carboxylate oxygen atoms are bridging tridentate, bonded two Cd atoms, forming a four-membered ring. (Such the carboxylic groups form

PS-07.04.34 THE STRUCTURE OF AQUOTETRACETANILIDE OF EDTA COBALT (II) PERCLORATE. By J. L. Briand$^1$, J. F. Piriella$^1$, A. Alvarez-Lorena$^1$, A. Namor$^2$, and J. Cardenas$^2$.

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In the context of a study on the use of Tetraacetanilide of EDTA for the recovery and purification of metals, we present here the X-ray crystal structure determination of the title compound. The crystallographic results show a coordination seven around the cobalt, one water molecule being coordinated with the metal.