

07-Crystallography of Organometallic and Coordination Compounds

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Cu(2+) with the carbon atoms of neighbouring molecules. In Cu(acetylacetonate)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 pseudodimeric and the second form of Y(dipivaloylmethanate)₃ is the dimeric one.

β -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 complexes". 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. Maxidentant 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 polyhedra 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 unclose-packed nets, having, for example, Schläfli symbols, 4⁴, 6³, 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 III has been shown to improve useful qualities of compounds.

PS-07.04.33 STRUCTURE OF GADOLINIUM COMPLEX WITH ACETYLENE DICARBOXYLIC ACID (ADA). By Yan Xing, Zhong-Sheng Jin, Zhi-Band Duan and Jia-Zuan Ni, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, People's Republic of China

Abstract Gd₂(ADA) · 8H₂O, Mr=794.8, triclinic, P $\bar{1}$, a=8.254(2), b=8.605(2), c=9.066(2) Å, α =95.38(2), β =115.82(2), γ =110.39(2)°, V=519.8(2) Å³, Z=1, D_x=2.54 g cm⁻³, λ (MoK α)=0.71069 Å, R=0.035 for 2694 observed reflections.

There are one and half ligands in an asymmetric unit. The molecular formula is Gd₂(ADA) · 8H₂O. The molecular structure is shown in Fig.1. The ligands are coordinated in three different forms in the molecule, firstly, 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 carboxyl bridge, presenting a double chain structure, thirdly, two carboxyl oxygen atoms are bridging tridentate, bonded two Gd atoms, forming a four membered ring. Such the carboxylic groups form

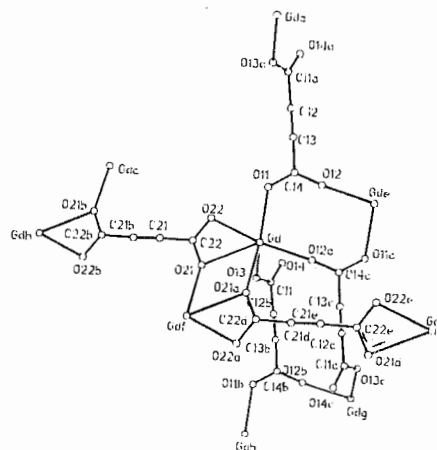


Fig.1. Molecular structure of Gd₂(ADA) · 8H₂O.

a single chain, which intersects the double chain above at each Gd atom, presenting a two dimension network structure. The Gd ion is 9-coordinate, bonded to six oxygen atoms from five carboxylic groups and to the three oxygen atoms of water molecules. There are two free water molecules in the unit cell. The Gd-O bond lengths range from 2.34 to 2.64 Å, one distance, namely, the Gd-O(21) of 2.64 Å, being significantly longer than the mean Gd-O bond length, 2.46 Å, the O(21) atom is the upper vertex of the tetragonal pyramid. The Gd-O(bridging bidentate) averaged distance of 2.35 Å is the shortest, but the Gd-O(chelating bidentate in bridging tridentate) averaged one of 2.50 Å is the longest in the three coordination forms. The rest Gd-O(water, unidentate, bridging part in tridentate) range from 2.42 to 2.49 Å with the mean bond length of 2.45 Å. The bond lengths and angles of the ADA in this paper are about the same as those of the literature(Allen and Don, 1973).

References

Allen, C.L., and Don, T.C.(1973). Acta Cryst. B29, 1579-1583.

PS-07.04.34 THE STRUCTURE OF AQUOTETRAACETANILIDE OF EDTA COBALT (II) PERCHLORATE. By J.L. Briansó*¹, J.F. Piniella¹, A. Alvarez-Larena¹, A. Namor², and J. Cárdenas².

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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.