

07-Crystallography of Organometallic and Coordination Compounds

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PS-07.04.04

PLANAR OR TETRAHEDRAL COORDINATION IN Cu(II) COMPLEXES INDUCED BY Br SUBSTITUTION.

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The synthesis and characterization of several new copper(II) complexes with ligands derived from bromosalicylaldehydes and (substituted) anilines have been reported recently. Magnetic susceptibilities, vibrational and electronic spectra and diffraction studies show that the environment of Cu atom varies from planar to quasi-tetrahedral, depending on the substituent (Costamagna *et. al.*, *Coord. Chem. Revs.*, 1992, 119, 67-88; *Acta Cryst.*, 1990, C46, 1823-1826).

Two Cu(II) complexes have been synthesized and their structures determined by direct methods, Siemens package programs, 2 θ - θ scan and MoK α . The collected reflections were affected by systematic errors related to the diffractometer state. The reason for these errors are not yet understood. Most of the reflections showed flat profiles but only a few of them had $I < 3\sigma(I)$. With these data sets it was not possible to solve the structures. However, with profile fitted data it was feasible to do so.

Bis(3-bromo-N-m-tolylsalicylaldiminato)Cu(II), monoclinic P2₁/c; a=9.919; b= 10.965; c=12.283, Å; β = 105.88°; R_f = 0.064. The Cu atom is in a special position and shows a planar geometry.

Bis(3,5-dibromo-N-p-tolylsalicylaldiminato) Cu(II), monoclinic P2₁; two molecules per asymmetric unit; a=13.290; b= 12.195; c=17.891, Å; β =105.38°. In this case, the copper atom shows a marked distorted planar coordination.

PS-07.04.05 INTRA-MOLECULAR NITROGEN-

TELLURIUM COORDINATE INTERACTIONS. By T. A.

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Compounds of type RTeX (X = halogen) are generally reactive, but they may be stabilised by reduction of the Lewis Acidity of the tellurium atom by intra-molecular coordination (McWhinnie, *Phosphorus, Sulfur, and Silicon*, 1992, 67, 107). In this context we have been studying the intra-molecular binding interactions between Te and N donor atoms in a number of organotellurium (II) and tellurium (IV) compounds containing nitrogen atoms sterically capable of coordinating to the central tellurium atom. We now report the crystal structures of

2-BrTe(II). C ₆ H ₄ NH (p-tolyl)	(1)
(8-O-quinolyl) ₂ (p-tolyl) ₂ Te(IV)	(2)
(8-O-quinolyl) ₂ Me ₂ Te(IV)	(3)

The Te-N distance in (1) is 2.375 (13) Å, with bromine bonded to tellurium *trans* to the Te-N bond. This distance may be considered to indicate a significant bonding interaction. In (2) and (3), Te-N distances are in the range 2.8 - 2.9 Å, indicating a much weaker or, perhaps, insignificant interaction. Here the bond *trans* to Te-N involves in each case a carbon atom. Factors affecting the strength of the Te-N bonding will be discussed. These include the valence state of the N atom and the nature of the group attached to Te, *trans* to the putative Te-N bond.

PS-07.04.06

ARCHITECTURE OF CRYSTALS OF COMPLEXONATES WITH OUTER SPHERE CATIONS

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Based on CCSDB and our own X-Ray data we carried out the systematic analysis of the complexonates with outer sphere cations. For all considered compounds the main structure agglomerates were examined and classified by the manner of their construction. The graphs reflecting the topological features of the studied structures on the hyperatomic level were built. We showed that, depending on their polarizing ability and the configuration of the complexonate anion, outer sphere cations are able to perform one of the following structural functions: 1) The filling of empty space, which is the result of the formation of polymer complexonate fragment packing in crystal. 2) The surrounding of the formed anion fragments, which is accompanied by the increasing of the section of islands, chains or layers. 3) The formation of the connecting links between anion complexes. 4) The formation of oligo and polymer fragments (with the participation of donor atoms of the complexone), which are "independent" structural agglomerates. 5) The formation of the joint packing with the complex anions. In this case the primary bonds between outer sphere cations and complex anions are absent. Moreover, our attention was focused on the possibility of the retention of intermolecular secondary bonds M...O in considered crystals.

PS-07.04.07

STRUCTURE OF COMPLEXONATES OF COBALT BASED ON NITRILOTRIACETIC ACID AND ITS ANALOGS

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This work is devoted to the retrospective review of the crystal structures of cobalt complexonates with nitrilotriacetic acid and its analogs. The structures of 18 such compounds are presently known, of which 16 were solved with the participation of the authors of this work. Our attention is mainly focused on the consideration of the following aspects:

1. The preferential configuration of Co(II) and Co(III) complexes in monoamine complexonates
2. The calculation of chelate metalocycle conformations
3. The analysis of the statistics of angular and distant distortions of Co(II) and Co(III) coordinational polyhedra.
4. The influence of additional ligands on the character of the Co coordinational polyhedron distortion
5. The peculiarities of Co complex configurations and of the packing of complex units in the presence of outer sphere cations of alkali and alkali-earth metals.