

Coordination mode of the zinc(II) and cadmium(II) cations with N-(diisopropoxyphosphoryl)thiobenzamide

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Abstract

Reaction of the potassium salt of N-(diisopropoxyphosphoryl)thiobenzamide (iPrO)₂P(O)NHC(S)C₆H₅ (HL) with ZnII and CdII cations in aqueous EtOH leads to three different complexes: [Zn(L-O,S)₂] (1), [Cd₂(L-O,S)₄] (2) and [Cd(HL-O)₂(L-O,S)₂] (3). The structures of these compounds were investigated by single-crystal X-ray diffraction analysis, EI-MS and ES-MS, IR, ¹H, ¹³C and ³¹P NMR spectroscopy and microanalysis. The zinc(II) atom in complex 1 is in a distorted tetrahedral ZnO₂S₂ environment formed by the C=S sulfur atoms and the P=O oxygen atoms of two deprotonated ligands. The cadmium(II) complex 2 is centrosymmetric and consists of dimeric species. Two [Cd(L-O,S)₂] moieties are connected by two bridging [S-Cd-S] units through the sulfur atoms of the ligand C=S groups. Complex 2 has a distorted trigonal-bipyramidal Cd(Oax)₂(Seq)₃ core. Complex 3 has a tetragonal-bipyramidal environment, Cd(Oax)₂(O eq)₂(Seq)₂, and two neutral ligand molecules are coordinated in the axial positions through the oxygen atoms of the P=O groups. The base of the bipyramid is formed by two anionic ligands in a typical 1,5-O,S coordination mode. The ligands are in a trans configuration. © Wiley-VCH Verlag GmbH & Co. KGaA, 2006.

<http://dx.doi.org/10.1002/ejic.200501005>

Keywords

(Thioacylamido)phosphates, Cadmium(II) complexes, Chelates, Coordination modes, Crystal structures, Zinc(II)