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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, El-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.

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Keywords

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