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The influence of the intramolecular hydrogen bond on the 1,3-N,S- and 1,5-O,S-coordination of N-phosphory--N′-(R)-thioureas with Ni(II) and Pd(II)

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Abstract

Reaction of the potassium salts of N-phosphorylated thioureas of common formula R1-N(H)-C(--)-N(H)-P(O)(OiPr)2 (HA) with Ni II and PdII cations leads to [MA2] chelate complexes (M = NiII, R1 = p-MeOC6H4, p-BrC6H4, t-Bu, c-Hex; M = PdII, R = iPr). In both the NiII and PdII complexes, the metal center is found in a square-planar N2S2 environment formed by the C=S sulfur atoms and the P-N nitrogen atoms of two deprotonated ligands A -. The PdII atoms in [PdB2] complexes with deprotonated thioureas of common formula R2-C(S)-N(H)-P(O)(OiPr) 2 (HB) (R2 = Et2N, morpholine-N-yl) are coordinated in a square-planar fashion by the C=S sulfur atoms and the P=O oxygen atoms of two anionic ligands. Molecular structures of four complexes [M(A-N,S)2] (M = NiII, R1 = p-MeOC 6H4, p-BrC6H4, t-Bu; M = Pd II, R1 = iPr) and the palladium(II) 1,5-O,--chelate of formula [Pd(B-O,S)2] (R2 = morpholine-N-yl) were elucidated by X-ray diffraction. © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique.

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