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Synthesis and X-ray crystal structures of N,N,N',N'-tetraalkylpyridine-2,6-dithiocarboxamides (S-Title:

dapt) complexes of cobalt(II) and nickel(II)

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Five-coordinate X-ray crystal structure 6-Dithiocarboxamides

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Abstract:

Reactions of anhydrous CoX2 (X = Br-, SCN-) and Ni(ClO4)2 with N,N,N',N'-tetraisobutylpyridine-2,6-dithiocarboxamides (S-dbpt), N,N,N',N'-tetraisopropyl pyridine-2,6-dithiocarboxamides (Sdppt), and N,N,N',N'-tetraethylpyridine-2,6-dithiocarboxamides (S-dept) lead to the formation of [Co(S-dbpt)Br2] (1), [Co(S-dppt)(SCN)2] (2), and [Ni(S-dept)2] (ClO4)2 · H2O (3), respectively. The X-ray crystal structures of the three S-dapt ligands and three complexes along with spectroscopic analyzes are presented. The molecular structure investigations of the S-dapt ligands show that the thiamide planes are twisted with respect to the pyridine ring, which is more in the case of phenyl groups. The structures of the Co(II) complexes reveal that an increase in steric crowding on the amide side arms of the ligands has no substantial effect on the geometry adopted by the corresponding complexes. The Co(II) gives only 1:1 five-coordinate, ion-paired complexes with a distorted square pyramidal geometry. Ni(II), on the other hand, prefers an octahedral geometry with 1:2 metal-ligand ratio. The coordination behavior of S-dapt has been compared to the analogous oxo(O-daap) ligands. Lesser propensity of S atom to get involved in H-bonding interactions ensures an S-N-S type of tridentate coordination by S-dapt.

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