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Title:	Magneto-structural studies of two new cobalt(ii)-N,N- diisobutylisonicotinamide compounds: [CoLCl2]n and [Co(L) 2(H2O)4][CoLBr3] 2·2H 2O
Authors:	Kapoor, Ramesh (/jspui/browse?type=author&value=Kapoor%2C+Ramesh)
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Abstract:	Two similar synthetic pathways using the ligand N,N- diisobutylisonicotinamide (L) with anhydrous CoX2 salts (being X = Cl-, Br-) led to different species: a one-dimensional system, [CoLCl2]n, 1, and an ionic product [Co(L)2(H2O)4][CoLBr3] 2· 2H2O,2,respectively. Compound 1 is a polymer in which ligand L coordinates to tetrahedral Co II ions in a bidentate bridging fashion using the pyridine nitrogen and carbonyl oxygen atoms. Compound 2 consists of one octahedral cationic [Co(L)2(H2O)4] 2+ entity and two tetrahedral anionic [CoLBr3]- units. In this system, the ligand molecules coordinate only through the pyridine nitrogen atoms. The magnetic properties of 1 and 2 were investigated in the temperature range of 2.0 to 300.0 K and correlations between both (due to the existence of similar features) examined. The study of the magnetic properties of 1 was carried out by considering each Co II ion as a perfectly isolated system, hence, J = 0, but taking into account a significant zero-field splitting contribution due to distortions on the tetrahedral environment of the cobalt atoms. The fit of the magnetic susceptibility data together with reduced magnetization vs H/T measurements provided similar parameters (D = 10.8 cm -1, g1 = 1.92, g1 = 2.92 for the former and D = 11.04 cm -1and g = 2.05 for the latter, respectively). On the other hand, the magnetic response of compound 2 has been analyzed using a model which considers the presence of two tetrahedral and one octahedral Co(ii) ions (Co Td and Co Oh). The study was carried out in two separated blocks, above and below 80 K, where only the most significant effects at each interval of temperature were considered. As a result, the analysis of the magnetic data shows weak antiferromagnetic interactions between the Co Ohand the two Co Td ions (J = -0.41 cm -1) in 2. The best fit parameters were g CoTd = 2.89, g CoOh = 3.50, D CoTd = 10.62 cm -1, E CoTd = 2.95 cm -1, Δ = 240.9 cm -1 and J L-S = -107.1 cm -1, from where λ was calculated with a final value of -144.8 cm -1 (J L-S = Aκλ). The approximations performed to obtain these values provide reasonable results in agreement with compound 1 and also to other systems in the literature.
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