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Molecular Structures of Some Bivalent Metal Complexes of 1-(4-Acetylphenyl)imidazole and Co-Ligands

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Abstract:

A series of bivalent metal complexes having compositions $[\text{Co}(\mathbf{L})_2\text{Cl}_2](\mathbf{1})$, $[\text{Zn}(\mathbf{L})_2\text{Cl}_2](\mathbf{2})$, $[\text{Co}(\mathbf{L})_2(\text{H}_2\text{O})_4](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}(\mathbf{3})$, $[\text{Zn}(\mathbf{L})_2(\text{H}_2\text{O})_4](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}(\mathbf{4})$, $[\text{Co}(\mathbf{L})_2(\text{OAc})_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O} (\mathbf{5})$, $[\text{Mn}(\mathbf{L})_2(\text{OAc})_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O} (\mathbf{6})$, $[\text{Co}(\mathbf{L})_4(\text{NCS})_2](\mathbf{7})$, $\{[\text{Co}(\mathbf{L})_2(\mathbf{Fum})(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}\}_n (\mathbf{8})$ and $\{[\text{Mn}(\mathbf{L})_2(\mathbf{Fum})]\}_n (\mathbf{9})$ were synthesized using \mathbf{L} (\mathbf{L} = 1-(4-acetylphenyl)imidazole) and respective co-ligands. The mononuclear sets $\mathbf{1-2}$, $\mathbf{3-4}$ and $\mathbf{5-6}$ are isomorphous and isostructural in nature. Complex $\mathbf{7}$ is a mononuclear complex, $\mathbf{8}$ is a 1D coordination polymer and $\mathbf{9}$ is a 2D-coordination polymer. All the compounds were structurally characterized using IR spectroscopy, thermogravimetric analyses, powder X-ray and single crystal X-ray diffraction studies. In general, coordinated / lattice water molecules are found to be involved in O–H...O hydrogen bonding and counter ions, in other weak interactions like C–H...S, C–H...Cl and C–H...O. The aromatic ring of \mathbf{L} also is involved in C–H... π and π ... π stacking interactions. In $\mathbf{3}$ and $\mathbf{4}$, hydrogen bonding interactions between coordinated water molecules, lattice water and nitrate ion contain cyclic hydrogen-bonded architectures. In $\mathbf{5}$ and $\mathbf{6}$, acetyl group present in \mathbf{L} act as hydrogen bond acceptor through O...H–O interaction. In $\mathbf{8}$ and $\mathbf{9}$ \mathbf{Fum} coordinate to metal center in μ - η^1 : η^1 bidentate and μ_4 - η^1 : η^1 : η^1 : η^1 tetradentate fashions resulting in formation of 1D and 2D coordination polymers, respectively.

Keywords: π ... π stacking; O–H...O hydrogen bonding; imidazole; coordination polymer.

1. Introduction:

Design and synthesis of transition metal complexes with structural features have attracted much attention due to their intriguing architectures and topologies. Metal complexes have potential applications in the fields of magnetism[1-10], sensors[11-16], adsorption[17-21], catalysis[22-24], and ion-exchange[14,25-26]. The assemblies of metal complexes are not only governed by strong and highly directional coordination bonds but also directed by

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