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Four *N*-heterocyclic carboxylate-phenolate coordination compounds: Syntheses, structures, and fluorescent properties

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ABSTRACT Four coordination compounds, $Ca(dhpmca)_2(H_2O)_3$ (**1**), $M(dhpmca)_2(H_2O)_2$ (M = Mg (**2**), Mn (**3**)) and $Cu(dhpmca)(phen)(H_2O)\cdot NO_3\cdot H_2O$ (**4**) (Hdhpmca = 2,4-dihydroxypyrimidine-5-carboxylic acid, phen = 1,10-phenanthroline), were synthesized and structurally characterized. The structure analyses showed that compounds **1-4** feature mononuclear structures, where $dhpmca^-$ anions adopt carboxylate and phenolate groups to bind to metal centers in monodentate fashions. The other coordinated sites are occupied by the oxygen atoms from water molecules and the nitrogen atoms from phen molecules. In addition, compounds **1-4** were further extended by hydrogen bonding to afford a vast diversity of 3D and 2D supramolecular structures. Further study revealed that in addition to the ligand, the types and coordination configurations of the metal centers can also regulate the structures. Significantly, compounds **1-4** displayed the emission bands at 421 nm, 411 nm, 453 nm, and 442 nm, respectively, which virtually originate from intraligand π-π^* and n-π^* transitions.

KEYWORDS N-heterocyclic ligand, Carboxylate-phenolate, Coordination compound, Fluorescent property.

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