# Cadmium Carboxylate Chemistry: Preparation, Crystal Structure, and Thermal and Spectroscopic Characterization of the One-dimensional Polymer $[Cd(O_2CMe)(O_2CPh)(H_2O)_2]_n$

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Compound $[Cd(O_2CMe)(O_2CPh)(H_2O)_2]_n$ (**1**) was initially obtained in a serendipitous way during efforts to prepare a $Cd^{II}/PhCO_2^-$/bepy complex (bepy = 2-benzoylpyridine). With the identity of **1** established by single-crystal X-ray crystallography, a rational preparative route to this complex was designed and carried out by reacting $Cd(O_2CMe)_2 \cdot 2H_2O$ with a slight excess of PhCOOH in MeCN under reflux. The crystal structure of **1** consists of isolated zig-zag chains. The $Cd^{II}$ atom is coordinated to five carboxylate and two aqua oxygen atoms creating a distorted, capped trigonal prismatic coordination polyhedron. The acetate group exhibits the $\eta^1{:}\eta^2{:}\mu_2$ coordination mode, while the benzoate ligand is chelating. There is an extensive hydrogen-bonding network which reinforces the chains and also links them generating sheets. The new complex was characterized by IR, far-IR, Raman, CP MAS and solution $^{113}Cd$ NMR spectroscopy. The spectroscopic data are discussed in terms of the nature of bonding and the known structure. An anhydrous compound with the empirical formula $Cd(O_2CMe)(O_2CPh)$ was isolated during the thermal decomposition of **1**; the vibrational study of this thermally stable intermediate supports an 1D polymeric structure with 6-coordinate $Cd^{II}$ ions.

*Key words:* Cadmium Carboxylate Complexes, $^{113}Cd$ NMR Spectroscopy, Mixed Acetate-benzoate Complexes, Thermogravimetry, Vibrational Spectroscopy