Cadmium Carboxylate Chemistry: Preparation, Crystal Structure, and Thermal and Spectroscopic Characterization of the One-dimensional Polymer \([\text{Cd(O}_2\text{CMe})(\text{O}_2\text{CPh})(\text{H}_2\text{O})_2]_n\)

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\textit{In dedication to the late Professor John M. Tsangaris for his important contributions to Inorganic Chemistry}

Compound \([\text{Cd(O}_2\text{CMe})(\text{O}_2\text{CPh})(\text{H}_2\text{O})_2]_n\) (I) was initially obtained in a serendipitous way during efforts to prepare a \(\text{Cd}^{II}/\text{PhCO}_2^−/\text{bepy complex (bepy = 2-benzoylpyridine). With the identity of I established by single-crystal X-ray crystallography, a rational preparative route to this complex was designed and carried out by reacting Cd(O}_2\text{CMe})_2·2\text{H}_2\text{O with a slight excess of PhCOOH in MeCN under reflux. The crystal structure of I consists of isolated zig-zag chains. The Cd}^{II} \text{ 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 \text{ 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}\text{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}_2\text{CMe})(O}_2\text{CPh) was isolated during the thermal decomposition of I; the vibrational study of this thermally stable intermediate supports an 1D polymeric structure with 6-coordinate Cd}^{II} \text{ ions.}

\textit{Key words:} Cadmium Carboxylate Complexes, \(^{113}\text{Cd NMR Spectroscopy, Mixed Acetate-benzoate Complexes, Thermogravimetry, Vibrational Spectroscopy}