

## A Co-Crystallised Cobalt(II) Cluster of Pyridinedicarboxylic Acid (PDC) as a Luminescent Material for Selective Sensing of Methanol

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### Abstract

A luminescent Cobalt(II) co-crystal  $[\text{Co}_{13}(\text{PDC})_{16}(\text{H}_2\text{O})_{24} \cdot 7\text{H}_2\text{O}] \cdot 1$  (where  $\text{H}_2\text{PDC} = 2,6$ -pyridinedicarboxylic acid) have been prepared by oven-heating and slow evaporation of solvent. Single crystal X-ray diffraction (SCXRD) analysis revealed that **1** is a mixture of complexes that crystallizes in the triclinic space group P-1 and the geometry around the Co(II) ions is octahedral. The structure is extensively imbued with hydrogen bonding that helps in stabilizing the complex. Thermogravimetric analysis indicates that **1** is thermally stable up to 364 °C. The luminescence properties of **1** revealed a strong emission centered at 437 nm ( $\lambda_{\text{ex}} = 345$  nm) assigned to ligand to metal charge transfer (LMCT). The luminescence sensing of **1** towards volatile organic molecules were also examined. However, **1** displayed a turn off towards methanol compared to other molecules with high quenching efficiency and low limit of detection ( $3.5 \times 10^{-4}$  vol%). The results show excellent selectivity and high sensitivity. Powder X-ray diffraction studies revealed that the structural integrity of the complex was maintained after exposure to methanol vapour. Theoretical studies also revealed small binding energy (-413.2 au) and low energy gap (1.19) for **1**-CH<sub>3</sub>OH adduct.