Theoretical and spectrochemical studies of cobalt oligonuclear hybrid materials with amino alcohols

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Oligonuclear and polynuclear transition metal complexes have been at the forefront of advanced materials coordination chemistry, because of the broad spectrum of applications in catalysis, nanoscience, optoelectronics, magneto-optics, and the biological-environmental field.[1,2] Among those metal ions, cobalt attracts considerable attention due to its chemical reactivity with appropriately configured (O,N,O)-terminal containing amino alcohol ligands. Design, synthesis, and optimization of the specific metal-organic systems in this study have been investigated synthetically based on the a) composition, involving ternary partners (aromatic chelators), such as 2,2'-bipy and 1,10-phen, b) molecular stoichiometry, c) temperature of the reaction, d) solvent system, and e) temperature of isolation (4-25 ^{o}C). Successful isolation of six compounds of the investigated ternary systems, based on Co(II) and iminodipropanol in methanol, reveals that there is a temperature-specific trend in the chemistry of the reagents employed, when it comes to the assembly of cluster species isolated in crystalline form and discrete phase. The isolated crystalline materials were characterized physicochemically by elemental analysis, FT-IR, UV-Visible, Photoluminescence, TGA, X-ray crystallography, EPR, and magnetics. Theoretical studies through Hirshfeld analysis were also carried out extensively. Collectively, the work proves that full optimization of cluster metal-organic assembly and distinct chemical reactivity is linked to reaction conditions, carefully introduced so as to lead to new well-defined hybrid metal-organic materials.

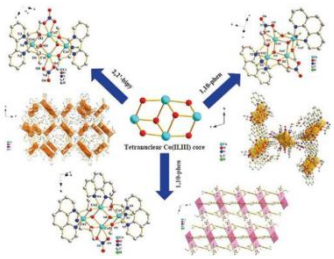

Figure 1: Tetranuclear cobalt clusters.

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