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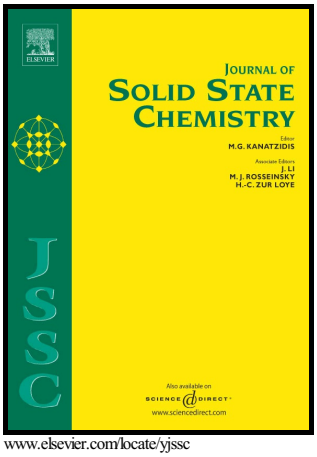

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Two-fold interpenetrating btc based cobaltous coordination polymer: a promising catalyst for solvent free oxidation of 1-hexene

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Abstract

This work describes the synthesis of a new 2-D coordination polymer (CP), $[Co_3(btc)_2(dmp)_8]_n$ (btc = 1,3,5-benzenetricarboxylate and dmp = 3,5-dimethylpyrazole) and its catalytic activity towards the oxidation reaction of 1-hexene to form oxygenated compounds under solvent free condition. Structural analysis reveals that Co(II) cations in this polymeric compound are linked by btc^{3-} anions with alternate tetrahedral/octahedral coordination forming a two-fold interpenetrated 3-connected **hcb** underlying net. Electronic spectrum of the cobaltous polymer has been calculated using TDDFT/B3LYP method for making the appropriate assignments of electronic transitions. Catalytic results show good conversions of the starting material to oxygenated products with high selectivities for 1,2-epoxyhexane and 1-hexanal.

Graphical Abstract

A new btc based 2-D coordination polymer of Co(II) has been synthesised solvothermally. Structural analysis reveals the presence of interpenetrating 3-coordinated **hcb** underlying nets in the crystal structure of the CP. This polymer is also found to be an excellent candidate towards the conversion of 1-hexene to various oxygenated products with high selectivity under solvent free condition.