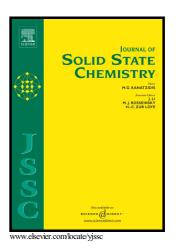
Author's Accepted Manuscript

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

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PII: S0022-4596(17)30341-9

DOI: http://dx.doi.org/10.1016/j.jssc.2017.08.034

Reference: YJSSC19924

To appear in: Journal of Solid State Chemistry

Received date: 9 July 2017 Revised date: 11 August 2017 Accepted date: 24 August 2017

Cite this article as: Sanchay J. Bora, Rima Paul, Mithun Nandi and Pradip K. Bhattacharyya, Two-fold interpenetrating btc based cobaltous coordination polymer: a promising catalyst for solvent free oxidation of 1-hexene, *Journal of Solid State Chemistry*, http://dx.doi.org/10.1016/j.jssc.2017.08.034

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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), [Co₃(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 btc³⁻ 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.

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