Poster Presentation

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Halide-bridged Polymers of d^{1°} Metals with Heterocyclic Type Donor Ligands

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Molecular self-assembly of organic ligands and inorganic metal halides leads to the formation of layered nano-composite organicinorganic hybrid materials. The formation of both ionic- and coordination hybrids is possible. Both of these materials have attracted much attention recently in the field of Crystal Engineering [1], due to the retention and combination of desired inherent properties of both constitutional moieties, which then renders these materials multifunctional with a wide range of potential technological applications. Properties attributed to the organic component include structural diversity and optical properties [2], with mechanical hardness, electronic-, magnetic- and optical properties ascribed to the inorganic component. The coordination of an organic amine functionality to a metal halide results in the formation of halide-bridged polymers coordinated to donor ligands, with reported properties including non-linear optic (NLO) behavior, magnetic properties [3] and electronic semi-conduction. Literature confirms the technological importance of these materials and identifies the need for research aiming at a fundamental understanding of factors that control the observed structural trends and to relate chemical composition and topology of these compounds to ultimately enable retrosynthesis from desired property. In this study, a range of different divalent d¹° metal halides are combined with different aromatic nitrogen-containing organic ligands. The effects of change in metal atom, halide atom, stoichiometry and reaction conditions on the structural trends in the crystal systems are investigated. The molecular self-assembly of the said halide-bridged polymers is initiated by simple synthetic techniques under relatively mild conditions, at the most, hydrothermal reaction conditions. Structural characterisation was done employing single crystal X-ray diffraction, while bulk composition of the samples was investigated using powder X-ray diffraction.

[1] G.M.J. Schmidt, Pure Appl. Chem., 1971, 27, 647-678., [2] D.B. Mitzi, D. Chondroudis, C.R., Kagan, IBM J. Res. & Dev., 2001, 45, 29-45., [3] D.M. Ciurtin, Y –B. Dong, M.D. Smith, T. Barclay, H-C zur Loye, H-C. Inorg. Chem., 2001, 40, 2825-2834.

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