Compounds of organic molecules and metal halides: structures and properties

Melanie Rademeyer, David C. Liles, Gerhard Overbeek, Stefan Coetzee, Department of Chemistry, University of Pretoria, Pretoria, (South Africa). E-mail: Melanie.rademeyer@up.ac.za

Organic molecules containing amine, carboxylic acid and/or amide functional groups may be combined with inorganic metal halides to form two different types of hybrid materials, both of which are of technological interest and self-assemble at the nano-scale.

When the components are combined as organic cations and perhalometalate anions, the resulting ionic-organic-inorganic hybrid material often retains the properties of the individual parts, with the inorganic component potentially contributing mechanical hardness, thermal stability, electronic properties (conductor, semiconductor, insulator) and magnetic properties, while the organic component may add structural diversity and optical properties (fluorescence and luminescence) [1]. Proven applications of these ionic hybrids include light emitting diodes (LED’s) [1].

Coordination compounds or coordination polymers are formed when the organic molecules coordinate to the metal atom of the metal halide component. The coordination polymers may be related to metal organic framework materials (MOF’s), and contain both organic linkers and inorganic halide linkers, whereas MOF’s typically only have organic linkers. Related coordination polymers have been reported to have interesting properties including non-linear optic behaviour and magnetic properties [2].

In the current study the effect of a change in one of the three parameters (organic component, metal atom and halide atom) on the crystal structures, packing and crystal engineering motifs are reported. In addition, the preliminary results of experimental properties, including band gap and electronic conduction, are presented, and compared to the properties calculated employing the software Materials Studio [3].

Keywords: crystal engineering, properties


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