

Imidazole-containing Co²⁺ and Ni²⁺ etidronates: crystal structures and electrochemical behaviour

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Abstract: Metal phosphonates-based coordination polymers (CPs) are known to exhibit versatile structural diversity and functionality [1]. Thus, they have been used, among other applications, as electrocatalyst precursors [2] for both, PEMFCs and electrolyzers.

In this work, we report the synthesis, crystal structure and electrochemical properties of imidazole-containing Co²⁺, Ni²⁺ and Zn²⁺ derivatives of the etidronic acid, (HO)₂P(O)-C(CH₃)(OH)-P(O)(OH)₂ (ETID). Analyses of the crystal structures reveals that these solids are 1D, in which the imidazole molecules form part of the coordination sphere of the cations (Co²⁺, Ni²⁺) or act as charge-compensating imidazolium cations (Zn²⁺). Co²⁺ and Ni²⁺ solids were pyrolysed under 5% H₂/Ar atmosphere at different temperatures. The resulting metal phosphides were tested as electrocatalysts for the Oxygen Evolution and Reduction Reactions (OER and ORR, respectively) and the Hydrogen Evolution Reaction (HER). Preliminary results indicate that Co²⁺ derivatives exhibit better performance.

Key words: Coordination polymers, phosphonates, imidazole, electrocatalyst, OER, ORR and HER.

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