Poster Presentation

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Carbonate contamination in nitrate and organic hydrotalcites by XRPD/TGA-GC-MS

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Layered double hydroxides are versatile materials used for intercalating bioactive molecules, both in pharmaceutical and cosmetic fields, with the purpose of protecting them from degradation, enhancing their water solubility to increase bioavailability, and/or obtaining modified release properties. The crystal chemistry of hydrotalcite-like compounds is investigated by X-ray powder diffraction (XRPD) and hyphenated TGA-GC-MS to shed light on the mechanisms involved in ion exchange and absorption of contaminants, mainly carbonate anions. XRPD demonstrated that the presence of carbonate is able to drive the intercalation of organic molecules into LDH, since CO3 contaminated samples tend to assume d-spacing roughly multiple of LDH-CO3 d-spacing. TGA-GC-MS allowed distinguishing and quantifying intercalated and surface adsorbed organic molecules, confirming the presence and amount of carbonate, especially at low (ppm) concentrations and separating the different types and strength of adsorption, in relation with the temperature of elimination. Also the importance of the intercalation method on the carbonate absorption was examined. This is probably due to the fact that the larger molecules leave some voids in the packing and the carbonate can occupy these voids during the intercalation. Finally the presence of adsorbed and not intercalated organic guest was quantified by TGA-GC-MS.

Keywords: Hydrotalcites, X-ray Powder Diffraction, TGA-GC-MS