Determination of the crystal structure of magnesium stearate hydrate using micrometre size single crystals

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Due to its anti-adherent and lubricating properties, magnesium stearate is the most used additive in pharmaceutical products [1]. Most products contain a few percent of magnesium stearate. The compound exists in several hydrated states, and the state of hydration has important consequences for the lubricating functionality [2]. Yet, none of the crystalline phases has been structurally determined despite the extensive use of this compound in pharmaceutical and other industries for over several decades [3]. The reason for that might be that commercially available samples are usually not pure; they contain a significant amount of magnesium palmitate – a stearate homologue differing by two CH2 groups. Furthermore, it seems to be problematic to obtain large enough single crystals suitable for a conventional X-ray diffraction experiment due to extremely low solubility of this material. We were able to synthesize highly pure magnesium stearate and obtain micrometre size single crystals suitable for a microdiffraction experiment at an X-ray synchrotron facility. The structure of magnesium stearate trihydrate could be determined (see Fig. 1). This is the first structurally characterized magnesium stearate hydrate phase. Our work could facilitate structure determination of other magnesium stearate phases as well those of magnesium palmitate from PXRD data. The structural data would be immensely useful to understand lubricating and other structure-determined properties of this extensively used material.

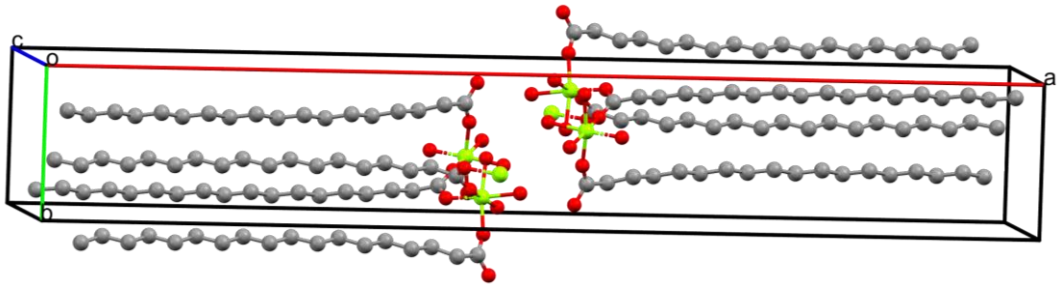

Figure 1. Packing representation of magnesium stearate trihydrate.

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