



## CRYSTAL STRUCTURE AND CHEMISTRY OF BARIUM-GRAPHITE INTERCALATION COMPOUNDS

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### ABSTRACT

Graphite can accommodate various chemical species between graphene layers to form graphite intercalation compounds (GIC) [1]. Alkali metals can easily lead to bulk stage-1 intercalation compounds by vapor transport but for more electronegative elements, such as alkaline-earth metals or lanthanides, only a superficial intercalation is obtained and other synthesis methods have to be envisaged. Molten alloys, formed between an alkali metal and the targeted metal, have demonstrated their efficiency to prepare bulk and homogeneous GIC from these latter elements, for example the superconducting  $\text{CaC}_6$  phase [2], but some elements remain difficult to intercalate by this method. More recently, our team developed a method based on the work of Hagiwara *et al.*, consisting in using a LiCl-KCl eutectic molten medium [3], which for example allowed to prepare for the first time a bulk  $\text{SrC}_6$  compound [4]. This work is focused on the intercalation of barium into graphite from the LiCl-KCl molten salts method. A bulk stage-1  $\text{BaC}_6$  compound has been prepared and X-ray diffraction measurements confirmed its crystal structure [5]. Moreover, by varying the experimental conditions, two completely novel phases, denoted  $\alpha$  and  $\beta$ , have been isolated. From ion beam analyses,  $\text{Li}_{0.2}\text{K}_{0.6}\text{Ba}_{0.35}\text{C}_6$  and  $\text{Li}_{0.2}\text{K}_{0.75}\text{Ba}_{0.6}\text{C}_6$  chemical formulae have been determined for  $\alpha$  and  $\beta$  phases, respectively, showing that lithium and potassium are intercalated together with barium. X-ray diffraction led to the determination of the stacking sequence of each compound, and their planar unit cells. Lastly, a reaction mechanism is proposed, which explains the formation of the different phases observed in this study.

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