Thermochemical modeling and synthesis of elements and compounds of groups 15 and 16 from the element oxides in [C4mim]BF4

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Innovative synthesis strategies for the formation of elements of group 15 (phosphorus, arsenic, antimony, bismuth) and group 16 (selenium, tellurium) or chalcogenides of group 15 metals for example Bi_2Te_3 can be realized by use of ionic liquids. This can be achieved both with and without using of an additional reducing agent.
Using complex CalPhaD modeling [1] and the resulting electromotive series of oxides according to SCHMIDT [2], rational synthesis planning can be carried out before the actual material synthesis. The electromotive series allows the clear representation of existence ranges $(p_i, E_i)_T$ of present compounds *i* and the assessment and prediction of the course of redox reactions (Fig. 1). In order to verify this theoretical approach, experiments with group 15 and 16 element oxides dissolved in the ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ($[C_4mim]BF_4$) were carried out by means of differential scanning calorimetry (DSC) with and without a reducing agent in a temperature range from −30 °C to 300 °C.
The values of the thermochemical stability (decomposition temperatures) of $[C_4mim]BF_4$ vary widely in the literature: from 360 °C [3] to 424 °C [4]. However, since the knowledge of thermal stability is essential for synthesis planning, the calculation of the maximum operation temperature (MOT) (Fig. 2) based on a kinetic model using non-isothermal TG-measurements has been performed before synthesis of investigated systems [5] [6].

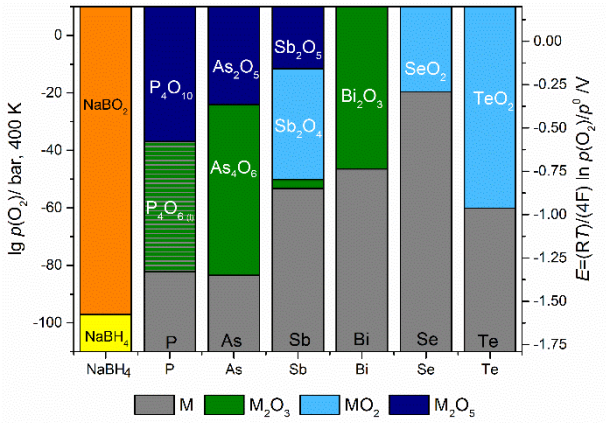

Figure 1: Electromotive series of solid oxides for the elements of groups 15 and 16, calculated at T = 400 K

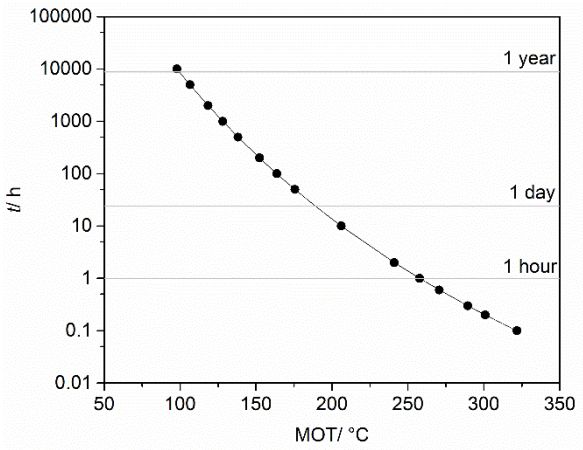

Figure 2: Calculation of the maximum operation temperature (MOT) of $[C_4mim]BF_4$ depending on the operating time

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