

Priority Programme

“Material Synthesis near Room Temperature”



Project Description – Project Proposal

Halogenated materials from novel reactive halogenating ionic liquids

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Summary of proposal

This project aims for the synthesis and characterization of novel reactive halogenating ionic liquids and their application in the synthesis of new halogenated materials. The halogenating reagents consist of polyhalogen anions with the general formula $[F(XF)_n]^-$ (with $X = \text{Cl, Br, I}$ and $n = 1-4$). With suitable cations these interhalide salts represent ionic liquids themselves or they are used with ionic liquids as liquefier. Due to the high solubility of gases and the weak interactions with the solute, ionic liquids represent ideal media for the synthesis and application of such polyhalogen monoanions. Furthermore they can be designed to be highly resistant towards strong oxidizers like Cl_2 , ClF and even elemental fluorine. The polyhalogen monoanions will be prepared by the reaction of naked F^- with halogenmonofluorides XF in suitable ionic liquids. Alternatively the reaction of polyhalide salts ($[\text{Cat}]^+[\text{X}(\text{X}_2)_n]^-$, $X = \text{Cl, Br, I}$ and $n = 1-4$) with F_2/N_2 mixtures will be investigated. Such interhalide salts dissolved in ionic liquids should be versatile halogenating reagents, which are safer and easier to handle than the gaseous, strong oxidizers ClF or F_2 . Due to their high heat capacity these are good media to moderate the usually quite exothermic halogenation reactions. For the synthesis of new materials we want to use these reactive ionic liquids especially in i) 1,1-addition and 1,2-additions, ii) halogene exchange reactions, and iii) $-\text{CN}$ to $-\text{CF}_3$ transformation. In particular efficient synthetic routes to the highly desired weakly coordinating closo-borate and closo-carborate anions like $[\text{B}_{12}\text{X}_{12}]^{2-}$, $[\text{CB}_{11}\text{X}_{12}]^-$ ($X = \text{F, Cl, Br, I}$) and the corresponding trifluoromethyl-substituted derivatives will be developed.