Priority Programme

“Material Synthesis near Room Temperature”

Project Description – Project Proposal

Synthesis of novel early transition metal cluster materials and polynuclear compounds using ionic liquids

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Summary of proposal

Polynuclear transition metal coordination compounds with (clusters) or without direct metal-metal bonds have attracted immense scientific and industrial interest for decades already. With the recently started eruption of activities with ionic liquids (ILs) this field seems to be jump-started again, because preliminary experiments indicate, that a multitude of novel compounds is available through the use of ILs in respective chemical reactions. Subject of this project is the designed synthesis and careful characterization of new and novel compounds of two classes of materials, A) compounds with hexanuclear cluster units of early transition metal atoms (M6-clusters) and B) Polynuclear coordination compounds of Cu, Cr/Mo, and Re. Using ILs as solvents and simultaneously as reaction components within the M6-cluster sub-project the synthesis and characterization of three groups of novel substances/reactions is proposed: 1) M6-clusters/chelate ligands: Using bifunctional ligands with the donor atoms separated by a benzyl-group shall allow for the synthesis of the first M6-cluster compounds with intra-cluster chelate ligands (M = niobium or zirconium). We expect these ligands strongly bonded, which is a prerequisite for complex compounds to be used as medical X-ray contrast agent. 2) In a second series of investigations, new fluoride-based cluster compounds are targeted. Within these, we plan in close cooperation with the group of Prof. I. Krossing (Freiburg) to attach polyfluoroalkoxy ligands to the cluster cores, expecting unprecedented weakly coordinating cluster anions. 3) In a third working package hydrogen atom containing cluster compounds are planned to be dissolved in ionic liquids and their ability to catalyze unsaturated organic molecules is tested. As soon as catalytic protocols are worked out, the extension towards the hydrogenation of formate and CO2 is planned. In the second sub-project B), novel Polynuclear coordination compounds of Cu, Cr/Mo, and Re are proposed to be investigated. Preliminary work, where simple starting compounds of the four metals were treated with acetate or azide based ILs, has shown that unprecedented novel coordination compounds of various nuclearities are accessible through this simple procedure using ILs. This chemistry will be continued and intensified within this project.