Density Functional Theory: Study on the Mechanism of the Chloride-Induced Aufbau of Perchlorinated Cyclohexasilanes

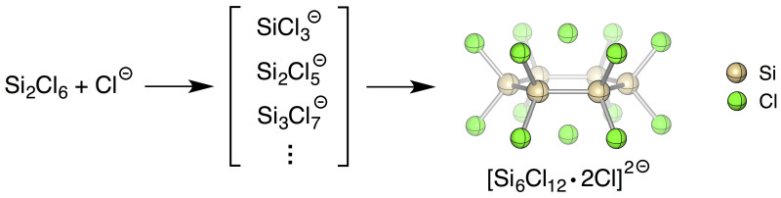


Fig. 1: Chloride induced formation of [Si6Cl12·2Cl]2-.

Introduction

Nano- and micrometer-scaled silicon structures are essential components not only in microelectronic but also in photovoltaic and opto-electronic applications. Oligo- and polymeric (perchloro)silanes are suitable precursors for the formation of silicon wires or thin silicon fi lms.

Methods

The mechanism of the amine-induced disproportionation of perchlorinated silanes aff ording neo-Si5Cl12 was recently established.[1,2] A surprisingly simple preparative procedure, the addition of Si2Cl6 to a solution of [nBu4N]Cl in dichloromethane, leads to the formation of a chloride-complexed cyclic dianion [Si6Cl12• 2Cl]2- and a variety of its silyl-substituted structural analogs, depending on the reaction conditions. The underlying reaction mechanism has been elucidated by DFT calculations (Fig. 1).

Results

It reveals the chloride ion itself as a Lewis base to trigger a disproportionation of perchlorinated silanes with a subsequent buildup of dianions containing up to eight silicon atoms.[3]

Outlook

The mechanistic insights gained provide the fundament required for the targeted synthesis of oligosilane precursors suitable for microelectronic applications.

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Clusters
LOEWE CSC Cluster Frankfurt

Institute
Institut für Anorganische und Analytische Chemie

University
Goethe Universität Frankfurt am Main

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TECHNISCHE UNIVERSITÄT DARMSTADT
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Reference

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[3] J. Tillmann, L. Meyer, J.I. Schweizer, M. Bolte, H.W. Lerner, M. Wagner, and M.C. Holthausen (2014), Chloride-Induced Aufbau of Perchlorinated Cyclohexasilanes from Si2Cl6: A Mechanistic Scenario, Chem.-Eur. J. 20, 9234-9239. https://doi.org/10.1002/chem.201402655

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