

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

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Clusters  
LOEWE CSC Cluster Frankfurt

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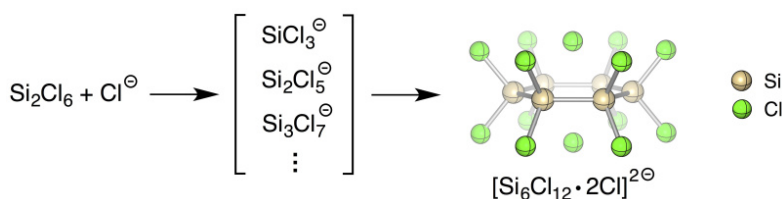


Fig. 1: Chloride induced formation of  $[\text{Si}_6\text{Cl}_{12}\cdot 2\text{Cl}]^{2-}$ .

## 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 films.

## Methods

The mechanism of the amine-induced disproportionation of perchlorinated silanes affording neo- $\text{Si}_5\text{Cl}_{12}$  was recently established.[1,2] A surprisingly simple preparative procedure, the addition of  $\text{Si}_2\text{Cl}_6$  to a solution of  $[\text{nBu}_4\text{N}]\text{Cl}$  in dichloromethane, leads to the formation of a chloride-complexed cyclic dianion  $[\text{Si}_6\text{Cl}_{12}\cdot 2\text{Cl}]^{2-}$  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.

## Reference

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