



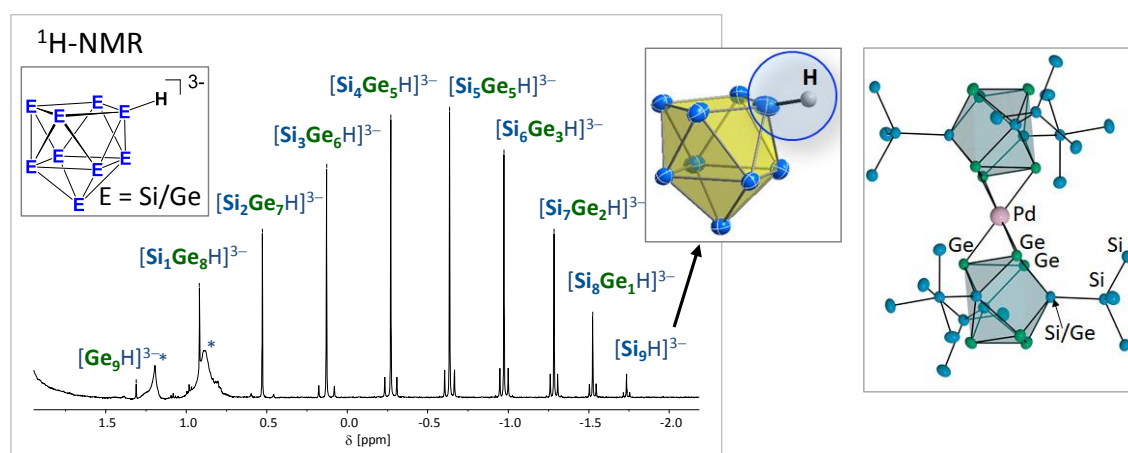
Direct Syntheses of Molecular Mixed Silicon-Germanium Compounds with Several Si-Ge bonds

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Many silicon allotrope semiconductor materials with a direct and quasi-direct band gap have been predicted,^[1] however, obtaining allotropes with a direct band gap through a chemical synthesis is difficult. Therefore research in the field to obtain suitable semiconductor materials with a direct band gap have focused also on semiconductor alloys such as Si-Ge. But in contrast to the elements Si and Ge that are fully miscible over the complete composition range $\text{Si}_{1-x}\text{Ge}_x$ ($0 \leq x \leq 1$) retaining the diamond structure with covalent bonds, molecules with several heteroatomic Si-Ge bonds that might serve as precursors are scarce.

After our successful attempts for the syntheses of bare Si clusters,^[2] we report now on the syntheses and isolation of a series of molecular clusters with mixed Si and Ge atoms. The nine-atom clusters can be obtained as protonated species $[\text{Si}_{9-n}\text{Ge}_n\text{H}]^{3-}$, as functionalized molecules of type $[\text{R}_3\{\text{Si}_{9-n}\text{Ge}_n\}]^-$ ^[3] and as metal complexes such as $[(^{\text{Me}}\text{Hyp}_3\{\text{Si}_2\text{Ge}_7\})_2\text{Pd}]^{2-}$.^[4]



The anionic molecules are spectroscopically characterized in solution by NMR and ESI-MS methods. The ^1H -NMR spectrum shows an unusual shift for the Ge-H and Si-H protons in the range of 0 ppm (Figure). In addition we report on the preferred functionalization of the clusters through the Si atoms and the coordination of such clusters to transition metals (Figure). Single crystal X-ray structure determinations allow for the allocation of Si and Ge atoms. In addition we report on the dynamic behavior of the mixed clusters through temperature dependent ^{29}Si -NMR measurements.

References

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