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## Mechanism of the hydrolysis reactions of 1-hydroxysilatrane and 1-hydroxygermatrane, 2,2-dihydroxysilocane and 2,2-dihydroxygermocane

Vereshchagina Y., Chachkov D., Alimova A., Ishmaeva E.  
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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### Abstract

© 2016 Taylor & Francis Group, LLC. The mechanism of the hydrolysis reactions of 2,2-dihydroxysilocane, 2,2-dihydroxygermocane, 1-hydroxysilatrane, and 1-hydroxygermatrane was studied by the density functional theory method. According to the quantum chemical calculations, the reactions of hydrolysis for 2,2-dihydroxysilocane and 2,2-dihydroxygermocane are characterized by the lower values of activation energy than for 1-hydroxysilatrane and 1-hydroxygermatrane. The ring configurations of the hydrolysis products are stable due to the presence of transannular interaction  $N \rightarrow X$  ( $X = \text{Si}, \text{Ge}$ ) and intramolecular hydrogen bond in their molecules.

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### Keywords

atrane, germocane, quantum chemical calculations, reaction mechanism, Silocane