Flash pyrolysis mechanism of trimethylchlorosilane

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The thermal decomposition mechanism of trimethylchlorosilane at temperatures up to 1400 K was investigated using flash pyrolysis microreactor coupled with vacuum ultraviolet (118.2 nm) photoionization time-of-flight mass spectrometry. The main initiation reaction of the parent molecule was identified to be HCl molecular elimination producing $Me_2Si=CH_2$. Other initiation pathways such as chlorine atom loss, methyl radical loss, or methane molecular elimination were also observed. Quantum chemistry calculations at the UCCSD(T)/cc-pVTZ//UM05-2X/aug-cc-pVDZ level of theory were performed to study the energetics of the possible initiation pathways. The theoretical calculations revealed that the HCl elimination channel via a van der Waals intermediate was the most energetically favored pathway among all the initiation channels, in agreement with the experimental observations. Secondary reactions of the initial products were identified, and the possible mechanisms were proposed.