

FLASH PYROLYSIS MECHANISM OF TRIMETHYLCHLOROSILANE BY FLASH PYROLYSIS VACUUM ULTRAVIOLET PHOTOIONIZATION TIME-OF-FLIGHT MASS SPECTROMETRY.

KUANLIANG SHAO, *Department of Chemistry, University of California, Riverside, Riverside, CA, USA*;
JONAH BRUNSON, *Department of Molecular, Cell and Systems Biology, University of California, Riverside, Riverside, CA, USA*; YI TIAN, *Department of Chemistry, Stony Brook University, New York, NY, USA*;
JINGSONG ZHANG, *Department of Chemistry, University of California, Riverside, Riverside, CA, USA*.

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 molecular elimination producing HCl and $\text{Me}_2\text{Si} = \text{CH}_2$. Other initiation pathways such as chlorine-atom loss, methyl radical loss, and methane elimination were also observed. Density function theory (DFT) calculations at UB3LYP/6-311++G(d,p) level of theory, with Grimme's empirical dispersion correction GD3, 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 initiation channels, in agreement with the experimental observations. Some secondary reactions of the initial products were identified, and their possible mechanisms were proposed.