

**In The Name Of Almighty God**

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**Shiraz University  
Faculty of Science**

**Ph. D. Thesis  
In Physical Chemistry**

**THEORETICAL STUDY ON THE KINETICS OF  
UNIMOLECULAR REACTION OF 1,2-  
DICHLOROETHANE AND BIMOLECULAR  
REACTION  $H + HOO$ , SYNTHESIS AND  
CHARACTERIZATION OF SILICON CARBIDE  
NANOSTRUCTURES**

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BY:

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**Dedicated**

**To My Wife**

*I would specially like to thank Dr. S. H. Mousavipour for his helpful and kindly advices during my studies. I thank Dr. A. Zeini Isfahani, Dr. A. H. Pakiari, Dr. M. H. Ghatee, Dr. A. Mohajeri and Dr. J. Moghadasi for reading the thesis and giving advices with writing it. My friends helped me with my study. I wish to thank Mr. Ramezani, Mrs. Homayoon and Mrs. Pirhadi and many other friends whose name are not brought here.*

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*Vahid Saheb*

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## Abstract

### Theoretical Study on the Kinetics of Unimolecular Reaction of 1,2-Dichloroethane and Bimolecular Reaction $H + HOO$ , Synthesis and characterization of Silicon Carbide Nanostructures

By

Vahid Saheb

Theoretical studies are performed on the kinetics of two reactions, unimolecular decomposition of 1,2-Dichloroethane and the reaction of atomic hydrogen with hydroperoxyl radical ( $HO_2$ ). Geometries, vibrational frequencies, and moments of inertia of all stationary points including reactants, transition states, energized intermediates and products are calculated by quantum mechanical methods.

RRKM theory is used to calculate the rate constants of unimolecular paths involved in decomposition of 1,2-Dichloroethane. The results show that the most dominant reaction is four-center HCl elimination reaction. Transition state theory is used to calculate the rate constants for those reaction channels of  $H + HOO$  reaction which proceed through a saddle point. The results from different levels of theory are reported for comparison.

On singlet potential energy surface, two reaction channels in  $H + HOO$  system proceed through potential wells. A TST-RRKM model is used to calculate the rate constant for these channels. It is concluded that most of atomic oxygen is formed through this intermediate on a singlet potential energy surface. Neglecting the formation of  $H_2OO^*$  causes the theoretical results do not agree with the experimental results.

Aside from theoretical kinetics studies, silicon carbide (SiC) nanostructures are synthesized by a magnesium-catalyzed chemical co-reduction route. Fourier transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), transmission electron microscope (TEM), and photoluminescence (PL) spectroscopy were used to characterize the gray product obtained. It is shown that well crystalline SiC nanorods is produced.

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# **Chapter 1**

**Introduction to the Kinetics of Unimolecular  
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Bimolecular Reaction  $\text{H} + \text{HOO}$**