

---

# **Ionization and fragmentation of chalcogene clusters by highly charged ions and synchrotron radiation**

---

**Inaugural-Dissertation  
to obtain the academic degree  
Doctor rerum naturalium (Dr. rer. nat.)**

**submitted to the  
Department of Biology, Chemistry and Pharmacy  
of Freie Universität Berlin**

**by  
Tiberiu Brebenel Arion  
from Agnita, Romania**

**Freie Universität**



**Berlin**

---

Berlin, April 2008

1. Gutachter: Prof. Dr. E. Rühl
2. Gutachter: Prof. Dr. E. Illenberger

Disputation am 22. Mai 2008

---

# Contents

<b>1</b>	<b>Introduction</b>	<b>9</b>
<b>2</b>	<b>Theoretical Background</b>	<b>11</b>
2.1	The Cluster Beam . . . . .	11
2.1.1	Sulfur . . . . .	13
2.1.2	Selenium . . . . .	14
2.2	NEXAFS Spectroscopy . . . . .	15
2.2.1	The Basic Principle . . . . .	16
2.2.2	Resonances at the Ionization Thresholds . . . . .	17
2.3	Basics of Model Calculations . . . . .	20
2.4	The Dynamics of Fragmentation . . . . .	22
2.4.1	Two-body Processes . . . . .	23
2.4.2	Three-body Processes . . . . .	25
2.4.3	Four-body Processes . . . . .	29
<b>3</b>	<b>Experimental Setup</b>	<b>33</b>
3.1	The Vacuum Systems . . . . .	33
3.1.1	The Oven . . . . .	35
3.2	Ionization Means . . . . .	36
3.2.1	Helium I Discharge Lamp . . . . .	37
3.2.2	Highly Charged Ion Beams . . . . .	38
3.2.3	Synchrotron Radiation . . . . .	40
3.3	The Detectors and The Spectrometers . . . . .	43

3.3.1	The Time-of-Flight Mass Spectrometer . . . . .	44
3.3.2	The COLTRIMS Reaction Microscope . . . . .	46
3.3.2.1	The Position Sensitive Detector . . . . .	48
<b>4</b>	<b>Results and Discussion</b>	<b>55</b>
4.1	Sulfur Cluster Investigation using HCI beams . . . . .	55
4.1.1	Mass Spectrometry . . . . .	58
4.1.2	Ion-ion-coincidence Spectroscopy . . . . .	64
4.1.2.1	$Xe^{5+}$ ion beam . . . . .	64
4.1.2.2	$Xe^{10+}$ ion beam . . . . .	70
4.1.2.3	$Xe^{15+}$ ion beam . . . . .	73
4.1.2.4	$Xe^{20+}$ ion beam . . . . .	77
4.1.3	Concluding Remarks . . . . .	84
4.2	COLTRIMS Investigations of Sulfur Clusters . . . . .	85
4.2.1	Identification of the Fragmentation Channels and Calibration . . . . .	86
4.2.2	Investigation of sulfur clusters as a function of the ionization energy . . . . .	89
4.2.3	Concluding Remarks . . . . .	93
4.3	Selenium Cluster Investigations . . . . .	93
4.3.1	Mass Spectrometry . . . . .	94
4.3.2	PEPIPICO Spectroscopy . . . . .	98
4.3.3	NEXAFS Spectroscopy . . . . .	102
4.3.4	Concluding remarks . . . . .	106
<b>5</b>	<b>Conclusions</b>	<b>111</b>
	<b>Bibliography</b>	<b>118</b>