

# Table of Contents

<b>List of Tables</b>	<b>xvii</b>
<b>List of Figures</b>	<b>xix</b>
<b>Abbreviations</b>	<b>xxv</b>
<b>1 An Overview</b>	<b>1</b>
1.1 Collision Processes and Energy Loss Mechanisms . . . . .	2
1.2 Plasmon or Collective Excitation . . . . .	3
1.3 Statistical and Non-statistical Decay Processes . . . . .	4
1.4 Theoretical Methods . . . . .	5
1.5 Experimental Techniques . . . . .	7
1.6 Polycyclic Aromatic Hydrocarbons and their Derivatives . . . . .	11
1.7 Electron-Ion Coincidence Measurements on PAHs and PANHs . . . . .	12
1.8 Thesis Outline . . . . .	14
<b>2 Theoretical Methodology</b>	<b>17</b>
2.1 Quantum Chemistry Calculation . . . . .	18
2.2 Structure Calculations . . . . .	20
2.3 Conclusion . . . . .	27
<b>3 Principles of Electron Spectroscopy and Ion Mass Spectrometry</b>	<b>29</b>
3.1 Requirements for Experimental Study . . . . .	30
3.2 Electron Spectrometers . . . . .	31

3.2.1	Retarding Field Energy Analyzer . . . . .	32
3.2.2	Parallel Plate Analyzer . . . . .	33
3.2.3	Cylindrical Analyzer . . . . .	35
3.2.4	Hemispherical Analyzer . . . . .	37
3.2.5	Toroidal Analyzer . . . . .	38
3.2.6	Time-of-Flight Energy Analyzer . . . . .	39
3.3	Ion Spectrometers . . . . .	41
3.3.1	Magnetic Sector Analyzer . . . . .	41
3.3.2	Quadrupole Mass Analyzer . . . . .	42
3.3.3	Time-of-Flight Mass Spectrometer . . . . .	43
3.3.4	Reflectron Time-of-Flight Mass Spectrometer . . . . .	45
3.4	Detection Systems . . . . .	47
3.4.1	Faraday Cup . . . . .	47
3.4.2	Channel Electron Multiplier . . . . .	48
3.4.3	Microchannel Plate Detector . . . . .	48
3.4.4	Position Readout . . . . .	51
<b>4</b>	<b>Experimental Methodology</b>	<b>55</b>
4.1	e, 2e Experiment . . . . .	56
4.2	Simulation and Design . . . . .	56
4.3	Electron Gun . . . . .	58
4.4	Electron Spectrometer . . . . .	60
4.5	Mass Spectrometer . . . . .	64
4.6	Pulsed Extraction ToF . . . . .	66
4.7	Projectile Energy Loss Analyzer . . . . .	68
4.8	High Voltage MOSFET Switch . . . . .	70
4.9	Electron and Ion Detectors . . . . .	72

4.10	Electron-Ion Coincidence Experimental Setup . . . . .	74
4.11	Fabrication . . . . .	75
4.12	Operational Modes of the Setup . . . . .	76
4.12.1	Electron Spectrum . . . . .	76
4.12.2	Mass Spectrum with Synchronized Switching . . . . .	78
4.12.3	Electron-Ion Coincidence Measurement . . . . .	79
4.13	Data Acquisition System . . . . .	80
<b>5</b>	<b>Testing and Calibration</b>	<b>83</b>
5.1	Testing for Vacuum . . . . .	83
5.2	Fast High Voltage MOSFET Switch Test for Electro-Optic Application .	85
5.2.1	Electro-Optic Modulator Experiment . . . . .	86
5.2.2	Calibration and Testing of Cylindrical Mirror Analyser . . . . .	91
5.2.3	Calibration and Testing of Time-of-Flight Mass Spectrometer . .	98
5.3	Multi Coincidence Experiment . . . . .	101
<b>6</b>	<b>Electron Impact on PAHs and PANHs</b>	<b>106</b>
6.1	Delayed Extraction Time-of-Flight . . . . .	108
6.2	DEToF Experimental Setup Details . . . . .	109
6.3	Analysis and Results . . . . .	111
6.3.1	Normalisation and Beam Energy Dependence . . . . .	116
6.3.2	HCN Loss Channel in Quinoline and Isoquinoline . . . . .	120
6.3.3	HCN+C <sub>2</sub> H <sub>2</sub> Loss Channel in Quinoline and Isoquinoline . . . .	121
<b>7</b>	<b>Ion Impact on PAHs and PANHs</b>	<b>125</b>
7.1	Experimental Details . . . . .	126
7.2	Mass Spectrum . . . . .	127
7.3	Plasmon Excitation in Charged Particle Collision . . . . .	134

7.4	Stability of PAHs and PANHs under Charged Particle Interaction . . . . .	142
7.5	Metastable Decay Dynamics of PANHs upon HCN Loss . . . . .	144
<b>8</b>	<b>Conclusion and Future Scope</b>	<b>147</b>
8.1	Instrumentation and Setup Development . . . . .	148
8.2	Calibration and Testing . . . . .	149
8.3	Investigation of Structural Effects in Napthalene and its Derivatives . . .	150
8.4	Future Scope . . . . .	151
<b>A</b>	<b>LUA Program Code Used in SIMION8.0 for Time Varying Electric Field</b>	<b>153</b>
<b>B</b>	<b>Arduino Program for Electron Spectrometer Operation and DAQ Automation</b>	<b>154</b>
<b>C</b>	<b>Function Fit Program for Metastable Decay Life-time Measurement</b>	<b>158</b>
	<b>Bibliography</b>	<b>159</b>
	<b>Publications Based on the Thesis</b>	<b>181</b>