

# Contents

<b>1</b>	<b>Kurzzusammenfassung</b>	<b>1</b>
<b>2</b>	<b>Abstract</b>	<b>3</b>
<b>3</b>	<b>Introduction</b>	<b>5</b>
<b>4</b>	<b>LIRTrap</b>	<b>7</b>
4.1	Setup of the 22-Pole Trap . . . . .	7
4.2	Mass Spectra . . . . .	11
4.3	Time Evolution of Chemical Reactions . . . . .	13
4.4	Spectroscopy via Laser Induced Reactions . . . . .	15
4.5	Daly Detectors for the New Ion Trap Experiments COLTRAP and FELion . . . . .	19
<b>5</b>	<b>Para Hydrogen</b>	<b>23</b>
5.1	Para Hydrogen Converter . . . . .	25
5.1.1	Production of Para Hydrogen in Continuous Flow . . . . .	26
5.1.2	Production of Para Hydrogen by Freeze Out . . . . .	28
5.2	Testing the Purity of Para Hydrogen with the Reaction $H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$ . . . . .	31
5.2.1	$H_3^+$ Isotopologues . . . . .	32
5.2.2	Theory . . . . .	32
5.2.3	Measurements in Continuous Flow Mode . . . . .	36
5.2.4	Measurements in Freeze Out Mode . . . . .	39
5.3	Testing the Purity of Para Hydrogen with Raman Spectroscopy . .	45
5.3.1	Raman Spectrometer . . . . .	45
5.3.2	Raman Measurements . . . . .	46
<b>6</b>	<b><math>N^+ + H_2 \rightarrow NH^+ + H</math>: Dependence of the Reaction on the Internal Energies of the Reaction Partners</b>	<b>55</b>
6.1	The $N^+ + H_2$ Reaction System . . . . .	56
6.2	Influence of the Temperature and the Ortho-to-Para Ratio of $H_2$ on the Reaction Rate . . . . .	58

6.3	Influence of the Fine-Structure of N <sup>+</sup> . . . . .	61
6.3.1	Fine-Structure of N <sup>+</sup> . . . . .	61
6.3.2	Ratecoefficients Including the Fine-Structure of N <sup>+</sup> . . . . .	62
6.3.3	First Experimental Results . . . . .	63
6.4	Influence of Different Experimental Parameters . . . . .	66
6.4.1	Influence of the Buffer Gas Density - Steps towards State-Specific Rate-Coefficients . . . . .	68
6.4.2	Effects of Different Ionization Energies on the Reaction System . . . . .	73
6.4.3	Influence of the Amplitude of the Trapping RF . . . . .	77
6.4.4	Conclusion on the Influence of Experimental Parameters. .	79
6.5	Results for the Purity of p-H <sub>2</sub> . . . . .	80
<b>7</b>	<b>Spectroscopy of CH<sub>2</sub>D<sup>+</sup></b>	<b>82</b>
7.1	The CH <sub>2</sub> D <sup>+</sup> Ion . . . . .	82
7.2	LIR Spectroscopy of CH <sub>2</sub> D <sup>+</sup> . . . . .	85
7.2.1	Production and Trapping of CH <sub>2</sub> D <sup>+</sup> . . . . .	86
7.2.2	Optical Parametric Oscillator . . . . .	86
7.2.3	Frequency Determination . . . . .	87
7.2.4	Spectra of CH <sub>2</sub> D <sup>+</sup> . . . . .	89
7.3	Spectroscopic Results . . . . .	89
<b>8</b>	<b>Line Profiles Observed with LIRTrap</b>	<b>92</b>
8.1	Theory . . . . .	92
8.2	Numerical Simulations with Python . . . . .	93
8.2.1	Simplified Model for Numerical Simulations . . . . .	94
8.2.2	Final Model for Numerical Simulations . . . . .	97
8.3	Test Measurements on CH <sub>5</sub> <sup>+</sup> . . . . .	105
8.3.1	Experiments on CH <sub>5</sub> <sup>+</sup> . . . . .	105
8.3.2	OPO System . . . . .	106
8.3.3	Fitting the Data . . . . .	106
8.3.4	Influence of the Number of Parent Ions . . . . .	108
8.3.5	Influence of the Laser Power . . . . .	114
8.3.6	Influence of the Time . . . . .	118
8.3.7	Influence of the Trap Temperature . . . . .	123
8.4	Conclusion on Line Profiles . . . . .	128
<b>9</b>	<b>Conclusion and Outlook</b>	<b>131</b>
<b>A</b>	<b>Appendix</b>	<b>140</b>
A.1	Python Simulation for LIR Line Profiles . . . . .	140
A.1.1	Main Program . . . . .	140
A.1.2	Frequency Dependence . . . . .	146

A.1.3	Time Dependence . . . . .	148
A.1.4	Write Results to File . . . . .	151
A.1.5	Plot Results . . . . .	153
A.1.6	Saturated Gaussian . . . . .	156
A.2	$\text{CH}_5^+$ Measurements . . . . .	157
A.3	Construction of the Readout Electronics Housing for the new Daly Detectors . . . . .	159
A.4	Production of p-H <sub>2</sub> . . . . .	170
A.4.1	Continuous Flow . . . . .	170
A.4.2	Freeze Out . . . . .	170
A.5	Fluctuations in Raman Spectra . . . . .	172
A.6	$\text{N}^+ + \text{H}_2$ . . . . .	174
A.6.1	Reactions with HD . . . . .	174
A.6.2	Effects of the Helium Buffer Gas . . . . .	175
A.6.3	Calibration of the RF Amplitude . . . . .	180