

# Preface

As this book contains my masters thesis, it is a summary of the insight I gained in the field of theoretical rovibrational spectroscopy of small molecules. It is more detailed and descriptive than a research article but certainly less educational than lecture notes or a textbook and this book should not be mistaken for any of these types of scientific texts. The way the methods are presented, however, should allow the reader to comprehend in detail the individual steps that were taken to obtain the results presented here. A more detailed understanding can be achieved with the aid of the standard textbooks and original research articles referenced within the text. The theory described in Chapter 2 and the Appendix should allow students of chemistry or physics and scientists that are new to the field to carry out their own calculations on similar systems and might help them to program their own rovibrational perturbation theory program. Astrochemists might be more interested in the results for the two linear interstellar molecules  $\text{l-C}_3\text{H}^+$  and  $\text{C}_4$ .

This work was realized only due to the help, knowledge and patience of my supervisor for more than two years: Prof. Dr. Peter Botschwina. Directly after my bachelor studies he offered me to work in his group as a research student and teaching assistant. During this time in Göttingen I had the chance to get a first insight into the scientific community, visit international conferences and get to know the process of scientific publishing. He offered all this generously while demanding nothing but an interest in science itself and his field in particular. There is no doubt that he fuelled my interest in theoretical chemistry and I am and always will be most grateful for his guidance and support. He died, rather unexpectedly, on December 27, 2014. His death is a great loss for the scientific community and the students but both have their invaluable memories.

I am grateful to my current supervisor Prof. Markus Reiher. He offered me a fascinating research topic that I enjoy working on every day and an environment that is extremely motivating. Furthermore, he recommended me for Springer's *Best Masters* series.

I also want to thank Prof. Ricardo Mata, who was the second referee for my thesis and a valuable advisor for many decisions I had to take.

Thanks are also due to my former colleagues Dr. Peter Sebald, Dr. Rainer Oswald, Benjamin Schröder, Arne Bargholz and Oskar Weser.

Studying science would be impossible (at least for me) without friends that find the right balance between motivating me and distracting me with non-scientific topics. In all stages of my life I had the luck to meet exceptionally great people and I am most grateful to all of you!

I deeply thank my family and especially my parents whose unconditional support and love are most precious to me! Without you, nothing I achieved in my life would have been possible.

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The Interstellar Molecules  $\text{l-C}_3\text{H}^+$  and  $\text{C}_4$

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