The anharmonic infrared spectra of polycyclic aromatic hydrocarbons

Mackie, J.C.

Publications

1. C. J. Mackie, T. Chen, A. Candian, X. Huang, T. J. Lee, and A. G. G. M. Tielens, Submitted (2018)

2. P. Castellanos, J. Bouwman, A. Candian, C. J. Mackie, H. A. Galue, D. Paardekooper, A. Petrignani, J. Oomens, H. Linnartz, and A. G. G. M. Tielens, Submitted (2018)

3. C. J. Mackie, T. Chen, A. Candian, X. Huang, T. J. Lee, and A. G. G. M. Tielens, Submitted (2018)

4. C. J. Mackie, A. Candian, X. Huang, E. Maltseva, A. Petrignani, J. Oomens, W. J. Buma, T. J. Lee, and A. G. G. M. Tielens, Phys. Chem. Chem. Phys. **20**, 1189 (2018)

5. E. Maltseva, A. Petrignani, A. Candian, C. J. Mackie, X. Huang, T. J. Lee, A. G. Tielens, J. Oomens, and W. J. Buma, Astron. Astrophys., Accepted (2018)

6. A. Candian and C. J. Mackie, Int. J. Quantum Chem **117**, 146 (2017)

7. C. J. Mackie, A. Candian, X. Huang, E. Maltseva, A. Petrignani, J. Oomens, A. L. Mattioda, W. J. Buma, T. J. Lee, and A. G. G. M. Tielens, J. Chem. Phys **145**, 084313 (2016)

8. E. Maltseva, A. Petrignani, A. Candian, C. J. Mackie, X. Huang, T. J. Lee, A. G. Tielens, J. Oomens, and W. J. Buma, Astrophys. J **831**, 58 (2016)

9. C. J. Mackie, A. Candian, X. Huang, E. Maltseva, A. Petrignani, J. Oomens, W. J. Buma, T. J. Lee, and A. G. G. M. Tielens, J. Chem. Phys **143**, 224314 (2015)

10. E. Maltseva, A. Petrignani, A. Candian, C. J. Mackie, X. Huang, T. J. Lee, A. G. G. M. Tielens, J. Oomens, and W. J. Buma, Astrophys. J **814**, 23 (2015)

11. C. J. Mackie, A. Candian, X. Huang, T. J. Lee, and A. G. G. M. Tielens, J. Chem. Phys **142**, 244107 (2015)

12. C. J. Mackie, E. Peeters, C. W. Bauschlicher Jr, and J. Cami, Astrophys. J **799**, 131 (2015)

13. L. S. Rothman, I. E. Gordon, Y. Babikov, A. Barbe, D. C. Benner, P. F. Bernath, M. Birk, L. Bizzocchi, V. Boudon, C. J. Mackie, et al., J. Quant. Spectrosc. Radiat. Transfer **130**, 4 (2013)

Curriculum Vitae

I was born on July 25th, 1984 in Toronto, Canada. Growing up I always had an interest in science, but not in an academic sense, rather in a trivial "fact" sense. I attended Seneca College briefly as a computer programming major. However, I could not find the drive or interest to continue down that path. I ended up working in IT for a number of years while deciding what my next step would be. This IT job required a lot of time killing, so I began to read more about the Sciences. Not just the "facts" that I always loved while growing up, but the actual philosophy of science. While reading about the Scientific Method it clicked for me. Science isn't *what* we know, its *how* we know. I knew at that instant that I did not want to just read about the findings of Science, I wanted to *do* Science.

After upgrading my education, I enrolled at the University of Waterloo as a Chemical Physics major. During my time as an undergraduate I fell in love with spectroscopy. It fascinated me how much we can learn about chemistry and matter just through measuring the light which it absorbs or emits. Specifically, I took a strong interest in the theoretical chemistry aspects of spectroscopy. Prof. Dr. Robert J. LeRoy graciously brought me into his group to work on a number of projects, including the electronic spectrum of xenon dimers. During my time with Bob, I was brought to a number of conferences. During one of these conferences I was introduced to Dr. Iouli Gordon.

At the time, Iouli wanted one of Bob's students to visit his group at the Harvard Smithsonian Center for Astrophysics for a summer to aide in research using a piece of Bob's software. At the CfA I worked on improving the spectroscopic line lists of molecular oxygen and carbon monosulfide. During my time at the CfA I further solidified my love of theoretical chemistry and spectroscopy, yet at the same time I extended my interests into astronomy. For my Masters I decided that I wanted to work in an astronomy department applying my spectroscopic knowledge to astrophysical problems. Iouli recommended Prof. Dr. Jan Cami as a supervisor at the University of Western Ontario.

I met with Jan and he hired me on for a masters project on characterizing the

infrared spectra of fully dehydrogenated polycyclic aromatic hydrocarbons. This was my first introduction to PAHs. Nearing the end of my masters, Jan brought me to the Netherlands for a conference on PAHs. Once again during a conference, I was introduced to my next supervisor Prof. Dr. Alexander Tielens. During the conference Xander questioned me about my plans after my Masters, and suggested that I come work with him for my PhD. Jan learned of what happened, and was not happy to lose me to Xander for my PhD (apparently Xander had to buy Jan a case of Belgian beer as an apology).

For my PhD I was supervised by Xander, Dr. Timothy J. Lee of NASA Ames, and Dr. Alessandra Candian. My PhD research (contained within this thesis) was on producing the anharmonic infrared spectrum of PAHs, in preparation for the unprecedented resolution that will be obtained by the James Webb Space Telescope (set to launch in 2019).

After completion of my PhD I will continue working in the field of theoretical chemistry, but I will be moving away from my astronomical ties. Instead I will be focusing on developing electronic structure theory methods to be used in theoretical chemistry calculations as a post-doc at the University of California Berkeley under the supervision of Prof. Martin Head-Gordon.

Acknowledgements

I would like to thank all of the people who made this thesis possible. Xander Tielens for providing me with the opportunity to pursue my PhD at Leiden University, and his invaluable supervision and research insight. Alessandra Candian for her advice, guidance and close collaborations. Tim Lee for providing supervision and advice with respect to the theoretical aspects of my work. Xinchuan Huang for his close collaborations, and providing deep understandings of the theoretical and computational aspects of my work. The experimentalists at the University of Amsterdam: Elena Maltseva, Wybren Jan Buma, and Annemieke Petrignani, who provided the experimental spectra, without which my work would not be possible. All of my additional collaborators and contributors to this thesis: Jos Oomens, Andy Mattioda, Pablo Castellanos Nash, Tao Chen, Jordy Bouwman, and Mieke Paalvast. My Observatory coffee mates: Allison Hill, Mason Carney, Mattia Fumagalli, Eva Bøgelund, and Nico Salinas. My office mates: Corentin Schreiber, Sascha Zeegers and Gilles Otten, Dario Campisi, Isabel Aleman, and Heather Andrews. The entire ISM group, namely Cornelia Pabst, Kirstin Doney, Pedro Salas Munoz, Kimberly Emig, Marcelo Leal-Ferreira, Lizette Guzman Ramirez, Daniel Harsono, Mher Kazandijian, Vincent Kofman, and Niels Ligterink. The Leiden University staff including Erik Deul and the ICT group, and Evelijn Gerstel and the financial and support staff. The Leiden faculty that I have interacted with over the years including Ewine van Dishoeck, and Harold Linnartz. Jan Cami for his supervision during my Masters, and continued support and friendship to this day. As well as, Neil Bhatt, Els Peeters, and Alexander DeSouza for their continued support and friendship. My NASA Ames colleagues who have always made me feel welcome during my visits: Partha Bera, Naseem Rangwala, Ella Sciamma-O'Brien, Lou Allamandola, Alessandra Ricca, Joe Roser, and Christiaan Boersma. My childhood friends which have been with me all these years: Robert Gallen, David King, and Michael Parkinson. My family for their unconditional support: Kathy Mackie and Garry Voisin, Charmaine and Marc Rosenberg, Elizabeth and Victor Iaccino, Cindy and Rob Wilson, and Kimberly Wilson and David Hutter. And most importantly my wife Kari, who followed me across the ocean so that I could pursue my dreams, provided unconditional love and support, and has given us our greatest accomplishment to date, Felix. One day I will teach all of this to you Felix.