Acknowledgements

To accomplish the journey of getting a doctorate in computational chemistry was not only working tirelessly a day via playing with a monitor and a sensitive keyboard. But, there were so many driving forces which constantly provided the motivation, maintained my will power and offered the energy to go forward feasibly and ultimately achieve my goal. These forces include all the well-wishers like my family, friends, colleagues, teachers and educational institutions where I was groomed primarily for achieving the goals independently. So at the culmination, all this beautiful bunch of people and places deserve recognition, appreciation and above all my gratitude for being an inspiration throughout my life and particularly in this triumph.

From the dawn of my life, it is my family who’s tireless and unconditional support, fortitude, rallying and unswerving loyalty and intimacy provided the broad substratum on which my whole life stands. The tolerance of my mischievous acts shows their resolute fidelity. I am overwhelmed by the faith they have shown in me and allowing me to follow my aims with my own attitude. I express my deep gratitude to my sisters: Ms. Roohi Jan and Ms. Neelofer Rasool for their unimaginable sacrifices towards my goals without which I could have existed nowhere in the road of my goals. Also, it is my father, Mr. Gh. Rasool Bhat and mother, Ms. Habla Begum who deserve a great applause and appreciation for their prudent attitude related to me due to which I always remained focused and thus attained a vision and impetus to move in the direction leading to my goals.

Before appreciating the galaxy of intellectuals, above all it is my Ph.D. supervisor, Dr. Prakash Chandra Jha, Chairperson, Centre for Applied Chemistry, Central University of Gujarat, India, to whom I would like to express my venerations and sincere gratitude for giving me a chance to perform the research work under his supervision. It is his kind supervision and guidance which drove me to face the challenges head on and overpower the snags. He induced a sense of independence in me and helped me to come out as an independent researcher. Falling short of words, I would like to mention that I am fortunate to be a part of his research group.

I would like to extend my wholehearted gratitude to Prof. Man Singh, Dean, School of Chemical Sciences, Central University of Gujarat, India, for finding me worth of the Ph.D. programme and selecting me for the course. I was overwhelmed by his staunch support he provided whenever, I approached his generosity. I was moved by his caring nature as he always looked like a family head.

I am highly indebted to Prof. R. K. Kale, former founder Vice-Chancellor of Cen-
tral University of Gujarat, for providing me a chance to become a part of this institution and providing the basic infrastructure particularly the computational resources.

I am grateful to the organizers of Central Universities Common Entrance Test-2013 for conducting all India Ph.D. programme entrance. It was this test through which I entered the domain of scientific research.

I am thankful to the University Grants Commission (UGC), Govt. of India, for providing the financial assistance which helped me to carry on my research smoothly.

I am highly thankful to UGC-Networking Resource Centre, School of Chemistry, University of Hyderabad, India, for arranging a training visit for me. The research presented in this thesis was partly carried out at School of Chemistry, University of Hyderabad, India, in the theoretical chemistry laboratory of an eminent scientist, Prof. Susanta Mahapatra. I am grateful to him for providing me some computational facilities.

I would like to extend my gratitude to all of my teachers from: a) Darakhshan Public School, Prichoo, Pulwama, J & K; b) Govt. Central Boys High School, Pulwama, J & K; c) Mehjoor Memorial Govt. Boys Higher Secondary School Pulwama, J & K; d) Govt. Degree College, Pulwama, J & K; e) Department of Chemistry, University of Kashmir, Hazratbal, Srinagar, J & K for their inspiration, motivation, encouragement, suggestions and above all transfer of knowledge which led me to achieve this degree.

I am highly thankful to the teaching and non-teaching staff of School of Chemical Sciences, Central University of Gujarat for their unending support and encouragement. These include: Dr. Dhananjay Mondal, Dr. Smritilekha Bera, Dr. Dinesh Kumar, Dr. Dandamudi, V. Lenin, Dr. Gururaja G. N., Dr. Panchami Prabhakaran, Dr. Vinod Kumar Singh, Mr. Bharat B. Rathod, Mr. Ashish Desai, and Mr. Biren B. Rathod.

I am very much thankful to my best friend Late Er. Mukhtar Ahmad Dar, for being the stalwart supporter whenever, I needed. I can’t forget his brotherly attitude towards me and of course treated me as a brother.

I would like to pay my thanks to all my relatives particularly my uncles- Mr. Gh. Mohiuddin Bhat, Mr. Abdul Gani Bhat, Mr. Mohd. Asan Bhat, Mr. Mushtaq Ahmad Bhat, Mr. Gulzar Ahmad Bhat; cousins- Mr. Shabir Ahmad Bhat, Dr. Mohd. Maqbool Bhat, Dr. Mohd. Yousuf Nengroo, Er. Ishfaq Ahmad Bhat, Mr. Riyaz Ahmad Bhat, Mr. Imtiyaz Ahmad Bhat, Mr. Showkat Ahmad Bhat, Mr. Naseer Gani, Mr. Adil Gani, Ms. Rifat Bashir, Ms. Afia Jan, Mr. Mushatq Ahmad Wani, Mr. Fayaz Ahmad Wani Mr. Yawar Mushtaq, Mr. Danish Mushtaq who took care of my family throughout these years when I was not present at home. I am particularly thankful to cousins- Dr. Mohd. Maqbool Bhat and Dr. Mohd. Yousuf Nengroo for their suggestions and inspiration which proved as a road map for this feat.
I pay my sincere gratitude to my labmates- Mr. Mohsin Yousuf Lone, Mr. Showkat Hassan, Mr. Mohd Athar, Mr. Prabodh Ranjan and Ms. Anu Manhas who kept me hopeful and helped me to stay strong during the tough times throughout these years. They really encouraged, motivated and boosted me with a moral support.

I am very much obliged to my batchmate and friend Mr. Gopal Avashthi for his encouragement, priceless suggestions, bringing positivity in me during my tough times and above all taking care of me (like my siblings do!) when I met an accident back in March 2016. Thank you Gopi for being the golden share of this journey.

I am highly indebted to all my batchmates, senior and junior research scholars and students of School of Chemical Sciences in particular and other schools and centres in general for their encouragement, fruitful suggestions and their good wishes. I am grateful to my roommates, Dr. Thounaojam Somokanta, Mr. Ashish Mundra and Mr. Ashish Raj for their overall support, encouragement and their consolation during my hard times. Thank you Soma Bhai for being there as an elder brother and as an inspiration.

I am highly thankful to my senior Mr. Nitin Kumar Sharma and Mr. Shantilal Mehetre for their support and brotherly care during my planning and making preparations to attend the international conference WATOC-2017.

I extend my gratitude to all of my friends and well-wishers who always crossed their fingers for my success and made themselves available whenever, I asked for a favour. The list is so big that it is impossible to mention all the names, but to name a few is unavoidable: Mr. Waseem Qadir, Mr. Sameer Gulzar, Mr. Tanveer Ahmad Malik, Mr. Mohd. Maqbool Bhat, Mr. Ab. Qayoom Mir, Mr. Younis Ahmad, Ms Rabia Gul, Mr. Feroze Ahmad Jagoo, Mr. Muzaffar Ahmad Sheikh, Mr. Saleem Ahmad Yatoo, Mr. Zahoor Ahmad Wani, Er. Umer Salam, Ms. Abida Akhter, Mr. Showkat Ahmad Akhoon, Mr. Arshid Ahmad Mir and so on.

My acknowledgements will look imperfect and incomplete to me without mentioning my betrothed Ms. Marifat Farooq. I am greatly beholden to her for encouraging me during my failures, bearing me as I am and being a part of this journey throughout. Thank you for being a solace always.

Haamid Rasool Bhat