Acknowledgements

This is one of the last and probably the most difficult part of the thesis to write. To tell in a few words of the people who influenced, guided and helped you while completing this thesis, would be far from justice to any one of them. So, this short text is my attempt to express my gratitude for these wonderful people.

Without the unrelenting support of my parents this thesis would never have been possible. I am at loss of words to thank them. My elder sister, Jyotishree has also been supportive all along.

Professor Gadre’s uncanny ability to motivate a Computer Science major to pursue a Ph. D. had what landed me here. When I joined for my masters in Pune University, I had never thought of pursuing a Ph. D. program here. But it just so happened that I landed up doing my final year project and then continuing for Ph. D. with Professor Gadre. Apart from all thats good of him, he has always given me the freedom to explore whatever I was interested into, though would quite often say “No time pass!”.

Many of the past and present members of TCG have made my work place full of fun and positive interaction. Anuja, Balanarayan, Jovan, Kiran, Milind, Rashmi, Ritwik and Yogendra, it is always wonderful to have you around especially when I have doubts in Chemistry! Balanarayan has always been a wonderful person to discuss with for new ideas. Never ending discussions on variety of topics with Anuja, Ritwik and Yogendra have been fun. Anuja and Ritwik have also helped me in finding many bugs in MeTA Studio and making it more usable in the process. Sunil has been helpful from day one when I joined here and has provided all the office assistance when ever
required. Drs. Ajay Limaye, K. Babu and Anant Kulkarni have helped me during my early years in TCG. I would particularly like to thank Ajay, Babu and their families for an unforgettable and warm stay with them during my visit to ANU, Canberra.

I would also like to express my gratitude towards Drs. Alistair Rendell and Andrey Bliznyuk for fruitful interaction during my stay at ANU, Canberra. Joseph, Ph. D. student with Alistair, helped me a lot and made a cheerful atmosphere at Fenner Hall.

I am also thankful to Dr. S. Manogaran from IIT Kanpur for useful discussions on computing Hessian and frequencies.

Finally, I would like to thank Dr. V. Sundararajan and C-DAC, Pune for their support. Without generous financial support from C-DAC and free access to their vast computing resources, this thesis would not be a reality.

V. Ganesh