Appendices

LIST OF PUBLICATIONS

1. "The Charge Transfer Limit of a Chemical Adduct: The Role of Perturbation on External Potential".
   Aabid Hamid, Atul Anand and Ram Kinkar Roy, *Phys. Chem. Chem. Phys.* **2017,** *19,* 10905-10912.

2. "Solvent Effect on Stabilization Energy: An Approach Based on Density Functional Reactivity Theory".
   Aabid Hamid and Ram Kinkar Roy, *Int. J. Quantum Chem.* **2019,** *119,* e25909.

3. "Correlation between Equilibrium Constant and Stabilization Energy: A Combined Approach Based on Chemical Thermodynamics, Statistical Thermodynamics and Density Functional Reactivity Theory".
   Aabid Hamid and Ram Kinkar Roy, *J. Phys. Chem. A.* **2020,** *124,* 1279-1288.

4. "Validation of Hammett's Linear Free Energy Relationship Through an Unconventional Approach".
   Aabid Hamid and Ram Kinkar Roy, *J. Phys. Chem. A.* **2020,** *124,* 5775–5783.

LIST OF CONFERENCES/WORKSHOPS/MEETINGS

1. Participated in Nascent Development in Chemical Sciences during 16th-18th October, 2015 at **BITS Pilani, Pilani Campus, Rajasthan, India.**

2. Attended **Q-Chem workshop** on 19th October 2015 at **BITS Pilani, Pilani Campus, Rajasthan, India.**

3. Participated and presented a poster entitled, "Profiles of Components of Stabilization Energy and Their Physical Implications" in the **20th CRSI National Symposium in Chemistry** during 3rd-5th February 2017 at **Gauhati University, Guwahati, India**.
   Aabid Hamid and Ram Kinkar Roy.

4. Participated and presented a poster entitled, "Understanding the Charge Transfer Limit of a Chemical Adduct" in the **North West Meeting on Spectroscopy, Structure and Dynamics (SSD-2017)** during 18th-19th March, 2017 **at BITS Pilani, Pilani Campus Rajasthan, India.**
   Aabid Hamid and Ram Kinkar Roy.

5. Participated and presented a poster entitled, "Variation of Stabilization Energy with the Solvent Polarity: An approach based on DFRT" in the International Conference on **Nano and Functional Materials – Interface between Science and Engineering (NFM-2017)** during 16^{th}-18^{th} November, 2017 at **BITS Pilani, Pilani Campus, Rajasthan, India.**
Aabid Hamid and Ram Kinkar Roy.

6. Participated and presented a poster entitled, "Solvent Effect on Stabilization Energy: An Approach based on DFRT" in the International Conference on **Frontiers at the Chemistry-Allied Sciences and Interface (FCASI-2018)** during 21^{st}-22^{nd} December, 2018 at **University of Rajasthan Jaipur, India.**
Aabid Hamid and Ram Kinkar Roy.

7. Participated and presented a poster entitled, "A DFRT Based Study on the Correlation of pk_a with Stabilization Energy" in **16^{th} Theoretical Chemistry Symposium (TCS-2019)** during 13^{th}-16^{th} February 2019 **at BITS Pilani, Pilani Campus, Rajasthan, India.**
Aabid Hamid and Ram Kinkar Roy.

8. Participated and presented a poster entitled, "Correlation between Equilibrium Constant and Stabilization Energy: A Combined Approach Based on Chemical Thermodynamics, Statistical Thermodynamics and Density Functional Reactivity Theory (DFRT)" in **FIRST-DAE Computational Chemistry Symposium (DAE-CCS-2019)** during 7^{th}-9^{th} November, 2019 at **Bhabha Atomic Research Centre (BARC) Mumbai, India.**
Aabid Hamid and Ram Kinkar Roy.

BRIEF BIOGRAPHY OF PROF. RAM KINKAR ROY

Dr. Ram Kinkar Roy is a Full Professor of Chemistry at Birla Institute of Technology and Science Pilani, Rajasthan. He received his Ph.D. degree from CSIR – National Chemical Laboratory, Pune in the year 1996. During his doctoral studies he worked with Prof. Sourav Pal in the research area of theoretical quantum chemistry. After his doctoral degree, he spent a year at National Chemical Laboratory, Pune, working with Prof. Sourav Pal as a Research Associate (CSIR). As a visiting post-doctoral fellow, he worked with Prof. Paul Geerlings for a year (1997-1998) at Vrije Universiteit Brussel, Belgium and also with Prof. Kimihiko Hirao in 1998-2001 at the University of Tokyo, Tokyo. He joined BITS Pilani, Pilani Campus in 2001. He was awarded JSPS and Senior JSPS Fellowship. He published several highly cited papers in reputed international journals. He completed three DST projects, and is presently dealing with the fourth one. Prof. Roy has successfully guided five Ph.D. students and is presently mentoring two students.

BRIEF BIOGRAPHY OF MR. AABID HAMID

Mr. Aabid Hamid, the author of the present thesis completed his Bachelors degree (B.Sc.) from University of Kashmir, Srinagar, India in the year 2011. He completed his Masters degree (M.Sc.) in Chemistry (with specialization in Physical Chemistry) from Jamia Millia Islamia (A Central University), New Delhi, India in the year 2013. In January 2015, he joined Ph.D. program in Prof. R. K. Roy's research group at BITS Pilani, Rajasthan. He worked in a DST-SERB project with Prof. R. K. Roy as Junior as well as Senior Research Fellow (DST-JRF & SRF). After successful completion of the project he was awarded Institute Senior Research Fellowship for almost two years. He has presented his work in several National and International conferences. He has published his work in several journals of international repute. Apart from research he was assigned as Instructor for both the experimental as well as the computational chemistry laboratory courses of B.E.-M.Sc. dual degree program.