PREFACE

The present dissertation entitled "THEORETICAL STUDY OF INTERACTION OF POLLUTANT IONS WITH WATER AND ORGANIC MOLECULES" is submitted to fulfill the requirements for the degree of Doctor of Philosophy (Science) of Jadavpur University. The thesis provides insight into structure, energetics, bonding, charge transfer and symmetry of arsenic cation-water cluster, as well as on structure, thermochemistry and bonding of complexes formed due to the interaction of group II b transition metal cations with nucleobases and 3-mercaptopropionic acid. A thermochemical study on arsine and its fluoro and chloro derivatives is also presented. All these studies are of environmental and toxicological interest and are accomplished by high-level theoretical methods. The investigations have been done under the supervision of Prof. Abhijit Kumar Das at the Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, West Bengal, India.

An introduction to the thesis is given in the first chapter to provide an idea about the environmental and toxicological chemistry. The second chapter briefly describes the computational chemistry and provides a review of theoretical methods. The remaining chapters of the thesis are based on the research papers published in reputed international journals. The original papers/manuscripts have been properly formatted to match the style of the thesis. Each chapter reviews the material presented in one (or two) published paper(s).

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