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Symposium on Computational Quantum Chemistry and Parallel Processors

University of Alberta, June 30 – July 2, 1986

Today's quantum chemists are in the position of the medieval traveller from the well-known woodcut reproduced on the cover who, after a long journey, peeks into the heavenly spheres. After many years of developing more and more sophisticated methods for handling complex chemical systems, we look into the future with hope that, before too long, it will be possible to perform calculations using the new, powerful computers which are currently emerging.

Up to the present, quantum chemical calculations were generally done on computers with "von Neumann", i.e. serial or scalar architectures. Such machines are in many ways inadequate to handle the kind and amount of computing which are typically required in applied quantum chemistry. Through the design of the new, more complex architectures, namely those of vector, parallel, and array processors, the speed and the power of computers are being greatly increased. For the full exploitation of these new hardware and software developments it will however be necessary to complement them by a rethinking and redesigning of the quantum chemical algorithms.

From June 30 through July 2, 1986, we invited about forty quantum chemists with a strong interest in the methodology of computations for a meeting to discuss responses to the new computer developments and to present new vistas in quantum chemistry. Almost thirty lectures and posters were presented. Some of them are published on the following pages.

We wish to express our gratitude to the Natural Sciences and Engineering Research Council of Canada, the Government of Alberta, the University of Alberta, the Department of Chemistry of the University of Alberta, and the Myrias Research Corporation who generously provided funds which enabled us to conduct the Symposium in a unique way. We also want to thank Dr. Zoila Barandiaran and Dr. Luis Seijo for their great help in running the Symposium.

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