
Preface

Proceedings of the XII Brazilian Symposium of Theoretical Chemistry

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This issue collects selected papers from the XII Brazilian Symposium of Theoretical Chemistry, held in the resort of Caxambu in the State of Minas Gerais, Brazil, during the period 23–26 November, 2003.

This symposium constitutes the major scientific meeting in the area of Quantum Chemistry and Molecular Physics in Latin America and has been organized every 2 years since 1981. This year we thus celebrate 20 years of an ever-increasing meeting, with strong and diversified participation that includes research seniors as well as students. In this version, over 360 participants, mostly from Brazil and South America, attended the meeting. The large number of groups around the country and the interchange of information between theoreticians and experimentalists created a unique environment for discussion of the scientific achievements of the last 2 years. Eighteen plenary lectures and 360 posters were presented dealing with different aspects of theoretical chemistry such as molecular spectroscopy, molecular modeling, catalysis, solvent and environment effects, biological systems, relativistic effects, molecular dynamics and Monte Carlo simulations, ab initio methods, high-performance computing, etc. Invited scientists from Argentina, Germany, Portugal, Sweden, and the United States contributed significantly to the success of this meeting in the form of plenary lectures and discussions. We warmly thank all of them.

The symposium paid tribute to the memory of our colleagues, and frequent participants, Prof. M. Giambiagi, a pioneer in the field of quantum chem-

istry, and Prof. Y.G. Smeyers, who acted many times as editor for previous proceedings.

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Finally, we thank the editors for the dedication and commitment in organizing the publication of these proceedings in the *International Journal of Quantum Chemistry*.

Organizing Committee of the XII Brazilian Symposium of Theoretical Chemistry: Kleber Mundim (UnB), Hélio Ferreira dos Santos (UFJF), Oscar Malta (UFPE), Hubert Stassen (UFRGS), Marco Antonio Chaer Nascimento (UFRJ), Antonio Carlos Borin (USP), Luiz Carlos Gomide Freitas (UFSCar), and Rogério Custodio (Unicamp).

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