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Preface

Special issue dedicated to Professor Erkki J. Brändas on the occasion of his 65th birthday

We are honored to be Guest Editors of this Special Issue of the *Journal of Mathematical Chemistry*. The primary focus has been to obtain papers with models and algorithms applicable to many different areas of mathematical chemistry. For example, we have contributions to modelling in the minimization of emissions in thermal plants, as well as in charge transport problems with quantum drift diffusion. We also have algorithms for improved parallel linear solvers, new filter techniques using finite Fourier transforms, minimization of non-smooth functions with applications in hydrothermal systems, new techniques for clustering and screening long-dimensional chemical data, and also higher order adaptive Runge-Kutta schemes for stiff problems. Finally the reader can learn how mathematical advances in signal processing through the fast Padé transform (FPT) greatly improves the information extracted via *in vivo* NMR chemistry.

We would like to very much thank Prof. Erkki J. Brändas, Uppsala University, for invaluable advice and assistance with the many aspects involved in producing a special issue like this. We also greatly appreciate the help and encouragement received from Prof. P.G. Mezey (Editor-in-Chief, JOMC) in editing this special issue.

We have asked Prof. Dzevad Belkic to write succinctly on Professor Erkki Brändas' achievements in science thus far, and here are the comments:

> Professor Erkki Brändas, as the former Head of the world-renowned quantum chemistry group from the Uppsala University (Sweden), and the current Executive Director of the Graduate Education Program for Advanced Instrumentation and Measurements proudly continues a great tradition initiated by Per Löwdin. This tradition is most known for the so-called Partitioning and Inner Projection Techniques which is a very important contribution to the establishment of computationally optimal intertwining of quantum-mechanical perturbation methods and variational principles for solving fundamental problems in physics, chemistry and beyond. The work of Professor Erkki Brändas abounds with rigorous mathematics of quantum mechanics ranging from fundamental operator formalisms to efficient computational algorithms that are critical to validation and application of any theory. In his publications, the most frequently used algorithms of Padé, Lanczos, Hankel, Stieltjes, Krylov, to name only a few of the mathematics masters, have systematically been highlighted from novel viewpoints both conceptually and computationally. His versatile activity and enviable success in research is being continuously conveyed to students and young scientists through his distinguished leadership at graduate studies at the Uppsala University. His expertise made significant contributions also to organizing or co-organizing many conferences in chemistry and physics, including those linking mathematical and computational methods within sciences and engineering which is the subject of this Special Issue of JOMC published under the auspices of CMMSE and devoted to Professor Erkki Brändas. It is the hope of all colleagues of

Professor Erkki Brändas, including myself, that his activity and, most importantly, his exemplary commitment to principle, both moral and scientific, will continue to inspire us and the generations to come.

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