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communications in mathematical
and in computer chemistry

Volume 60 (2008) number 3

A special section "*Numerical Methods in Chemistry*" edited by Theodore E. Simos and Charalampos Tsitouras

Foreword

- *C. Tsitouras, I. T. Famelis*: Quadratic SDIRK Pair for Treating Chemical Reaction Problems, pp. 697-710
- *H. Van de Vyver*: Efficient One-Step Methods for the Schroedinger Equation, pp. 711-732
- *Z. A. Anastassi, T. E. Simos*: New Trigonometrically Fitted Six-Step Symmetric Methods for the Efficient Solution of the Schroedinger Equation, pp. 733-752
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**Proceedings of the inaugural meeting of the
*European Society of Mathematical Chemistry,***

Cluj, October 23-26, 2007 (edited by Mircea V. Diudea)

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Latest News

17-01-2008

Photos from the conference can be downloaded [here](#).

04-09-2007

[Abstract template](#) is available. Please submit your abstracts prepared according to the template.

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Lecture and Poster Abstracts

Plenary Lectures

Lectures

Ali Reza ASHRAFI Computing PI Index of the Molecular Graphs of Nanostructures
Attila BENDE Hydrogen bonding in urea dimer and adenine-thymine DNA base pair: Anharmonic effects in intermolecular H-bond and intramolecular H-stretching vibrations
Vladislav BLATOV Generating periodic nets for crystal chemistry
Sorana BOLBOACA MODELING ANALYSIS OF AMINO ACIDS HYDROPHOBICITY
Ante GRAOVAC Some novel results on topological indices.
Ali IRANMANESH Computing the Szeged and PI indices of any graph By GAP program
Istvan LASZLO Topological coordinates for carbon nanotube junctions
Davide PROSERPIO Tilings and nets.
Mihai V. PUTZ Approximation Levels of the Quantum Chemical Bond and Bonding

Posters

Onisor CRISTINA Modeling and Prediction (Correction) of Partition Coefficients of Bile Acids and Their Derivatives by Multivariate Regression Methods
Badhin GÓMEZ VALDEZ Quantum Chemical Study of the Inhibitive Properties of 2-Pyridyl-Azoles
Lorentz JANTSCHI MOLECULAR DESCRIPTORS FAMILY PROJECT AND THEIR APPLICATION ON STRUCTURE-PROPERTY/ACTIVITY RELATIONSHIPS

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