

Institut "Jožef Stefan", Ljubljana, Slovenija

Jamova c. 39, 1001 Ljubljana, p.p. 3000 / Tel.: (01) 477 3900

Faks: (01) 251 93 85 / www.ijs.si



March 11, 2015

Aleksander Pavko, Editor
Acta Chimica Slovenica

Dear Editor,

Please find enclosed our manuscript entitled:

H-Bonded CH₃SO/H₂SO₄/H₂O Complexes: Quantum Chemical Study

by Simona Tušar and Antonija Lesar with a kind request to consider it for publication in *Acta Chimica Slovenica* as *Scientific articles* in the Special Issue Dedicated to Prof. Dr. Jože Koller on the occasion of his 70th birthday.

The scientists who would be competent to review the work critically and objectively:

- Agnie M. Kosmas, Univsity of Ioannina, Departant of Chemistry, Physical Chemistry Laboratory, GR-451 10 Ioannina, Greece;
E-mail: amylona@cc.uoi.gr
Position: Full Professor for Statistical Mechanics and Chemical System Dynamics at Physical Chemistry Section

1. Salta, Z.; Kosmas, A. M. Computational Study of the Reaction of the Methylsulfonyl Radical, CHS(O)₂, with NO₂, *Int. J. Quantum Chem.* **2014**, *114*, 1430-1437.
2. Kosmas, A. M.; Papayannis, D. K.; Tsiara, E. A computational study of the water-catalyzed reaction of chlornitromethane with the OH radical, *Comput. Theor. Chem.* **2013**, *1019*, 18-22.
3. Kosmas, A. M.; Mpellos C.; Salta, Z.; Drouga, E. Structural and heat of formation studies of halogenated methyl hydro-peroxide, *Chem. Phys.* **2010**, *371*, 36-42.

- Janez Mavri, National Institute of Chemistry, Laboratory for Biocomputing and Bioinformatics, Hajdrihova 19, 1000 Ljubljana, Slovenia;

E-mail: janez.mavri@ki.si

Positions/honors: (i) Head of the Laboratory for Biocomputing and Bioinformatics at the National Institute of Chemistry, Slovenia, (ii) Graduate course: Computer Aided Drug Design, Faculty of Pharmacy, University of Ljubljana, Slovenia (iii) Fulbright Scholarship, University of Southern California, USA

1. Pirc, G.; Stare, J.; Mavri, J.; Vianello, R. Hydrogen Bond Dynamics of Histamine Monocation in Aqueous Solution: How Geometric Parameters Influence the Hydrogen Bond Strength, *Croat. Chem. Acta* **2014**, 87, 397-405.
2. Vianello, R.; Mavri, J. Microsolvation of the histamine monocation in aqueous solution: the effect on structure, hydrogen bonding ability and vibrational spectrum, *New J. Chem.* **2012** 36 954-962.
3. Brela, M.; Stare, J.; Pirc, G.; Sollner-Dolenc, M.; Boczar, M.; Wojcik, M. J.; Mavri, J. CarParrinello Simulation of the Vibrational Spectrum of a Medium Strong Hydrogen Bond by Two-Dimensional Quantization of the Nuclear Motion: Application to 2-Hydroxy-5-nitrobenzamide, *J. Phys. Chem. B*, **2012**, 116, 45104518.

Yours sincerely,

Antonija Lesar

Corresponding Author:

Antonija LESAR

Institute Jožef Stefan

Jamova c. 39, P.O.B.3000

SI-1001 Ljubljana, Slovenia

Internet address: antonija.lesar@ijs.si

Tel. number: +386 1 477 3218

Fax number: +386 1 25 19 385