

ISSN: 2332-5968 Volume 6, Number 3, July 2018



Computational Chemistry



ISSN: 2332-5968



9 772332 596001 03

www.scirp.org/journal/cc

Journal Editorial Board

ISSN 2332-5968 (Print) ISSN 2332-5984 (Online)

<http://www.scirp.org/journal/cc>

Editor-in-Chief

Prof. Anwar El-Shahawy

Assiut University, Egypt

Editorial Board

Dr. Ali Khalaf Al-Matar

University of Jordan, Jordan

Dr. Enrique Arribas

University of Castilla-La Mancha, Spain

Prof. Nagarajan Arumugam

PSG College of Pharmacy, India

Prof. Todor Dudev

Sofia University, Bulgaria

Dr. Natalja Fjodorova

National Institute of Chemistry, Slovenia

Dr. Selseuk Gümüş

Yuzuncu Yil University, Turkey

Dr. Weiwei Han

Jilin University, China

Prof. Alireza Heidari

California South University, USA

Prof. Parasuraman Jaisankar

Indian Institute of Chemical Biology, India

Dr. Baiqing Li

Shandong University, China

Dr. C. Gopi Mohan

Amrita Institute of Medical Sciences and Research Center, India

Dr. Floriano Paes Silva Junior

Instituto Oswaldo Cruz, Brazil

Dr. Maurizio Sironi

University of Milan, Italy

Dr. Carlos P. Sosa

Cray Inc and University of Minnesota, USA

Prof. Hilal S. Wahab

Al-Nahrain University, Iraq

Dr. Carline Josette Weinberg

Roumanian Academy, Romania

Dr. Julliane Yoneda

Universidade Federal Fluminense, Brazil

Prof. Abdelkader Zarrouk

Mohammed First University, Morocco

Table of Contents

Volume 6 Number 3

July 2018

Molecular Structure, Electronic Structure, Properties and Analyses of Five Azopyridine Ruthenium Complexes α -Cl, β -Cl, γ -Cl, δ -Cl and ε -Cl of RuCl₂(4,6-Dimethyl-Phenylazopyridine)₂ as Potential Cancer Drugs: DFT and TD-DFT Investigations

N. K. N'Guessan, K. Bamba, O. W. Patrice, N. Ziao.....27

Conversion of 3,4-Dihydroxypyrrolidine-2,5-Dione to Maleimide through Tosylation and Mechanism Study by DFT

M. C. Yan, Z. Zhang, J. H. Zhou, W. Li, S. Fan, Z. Y. Yang.....47

Theoretical Study by Density Functional Theory Method (DFT) of Stability, Tautomerism, Reactivity and Prediction of Acidity of Quinolein-4-One Derivatives

A. L. Bédé, A. B. Assoma, K. D. Yapo, M. G.-R. Koné, S. Koné, M. Koné, B. R. N'Guessan, E.-H. S. Bamba.....57

Computational Chemistry (CC)

Journal Information

SUBSCRIPTIONS

The *Computational Chemistry* (Online at Scientific Research Publishing, www.SciRP.org) is published quarterly by Scientific Research Publishing, Inc., USA.

Subscription rates:

Print: \$39 per issue.

To subscribe, please contact Journals Subscriptions Department, E-mail: sub@scirp.org

SERVICES

Advertisements

Advertisement Sales Department, E-mail: service@scirp.org

Reprints (minimum quantity 100 copies)

Reprints Co-ordinator, Scientific Research Publishing, Inc., USA.

E-mail: sub@scirp.org

COPYRIGHT

Copyright and reuse rights for the front matter of the journal:

Copyright © 2018 by Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY).

<http://creativecommons.org/licenses/by/4.0/>

Copyright for individual papers of the journal:

Copyright © 2018 by author(s) and Scientific Research Publishing Inc.

Reuse rights for individual papers:

Note: At SCIRP authors can choose between CC BY and CC BY-NC. Please consult each paper for its reuse rights.

Disclaimer of liability

Statements and opinions expressed in the articles and communications are those of the individual contributors and not the statements and opinion of Scientific Research Publishing, Inc. We assume no responsibility or liability for any damage or injury to persons or property arising out of the use of any materials, instructions, methods or ideas contained herein. We expressly disclaim any implied warranties of merchantability or fitness for a particular purpose. If expert assistance is required, the services of a competent professional person should be sought.

PRODUCTION INFORMATION

For manuscripts that have been accepted for publication, please contact:

E-mail: cc@scirp.org

What is SCIRP?

Scientific Research Publishing (SCIRP) is one of the largest Open Access journal publishers. It is currently publishing more than 200 open access, online, peer-reviewed journals covering a wide range of academic disciplines. SCIRP serves the worldwide academic communities and contributes to the progress and application of science with its publication.

What is Open Access?

All original research papers published by SCIRP are made freely and permanently accessible online immediately upon publication. To be able to provide open access journals, SCIRP defrays operation costs from authors and subscription charges only for its printed version. Open access publishing allows an immediate, worldwide, barrier-free, open access to the full text of research papers, which is in the best interests of the scientific community.

- High visibility for maximum global exposure with open access publishing model
- Rigorous peer review of research papers
- Prompt faster publication with less cost
- Guaranteed targeted, multidisciplinary audience



Website: <http://www.scirp.org>

Subscription: sub@scirp.org

Advertisement: service@scirp.org