

PURE AND APPLIED CHEMISTRY

IUPAC PRESIDENT *Christopher Brett* (Portugal)
VICE PRESIDENT *Javier Garcia Martinez* (Spain)
PAST PRESIDENT *Qi-Fend Zhou* (China/Beijing)
SECRETARY GENERAL *Richard Hartshorn* (New Zealand)
TREASURER *Colin Humphris* (UK)

COMMITTEE ON PUBLICATIONS AND CHEMINFORMATICS DATA STANDARDS (CPCDS)

Leah McEwen (USA, chair); *James Liu* (USA, secretary); *Greg Banik* (USA); *Ian Bruno* (UK); *Stuart Chalk* (USA); *Jeremy Frey* (UK); *Wolfram Koch* (Germany); *Carmen Nitsche* (USA); *Kounosuke Oisaki* (Japan); *Ethel Rios-Orlandi* (Puerto Rico); *Rusli Daik* (Malaysia); *Margherita Gavagnin* (Italy); *Supa Hannongbua* (Thailand)

EDITORIAL ADVISORY BOARD

Richard Hartshorn (New Zealand, IUPAC Secretary
General, Acting Chair)

Mark Cesa (USA)
Nicole Moreau (France)
Natalia Tarasova (Russia)
Kazuyuki Tatsumi (Japan)
Pietro Tundo (Italy)
Qi-feng Zhou (China/Beijing)

Roger Hiorns (France), Polymer
Zoltán Mester (Canada), Analytical Chemistry
Yehuda Shevah (Israel), Chemistry and the Environment
Rita Cornelis (Belgium), Chemistry and Human Health
Alan Hutton (South Africa), Chemical Nomenclature and
Structure Representation

IUPAC DIVISION REPRESENTATIVES

Ron D. Weir (Canada), Physical and Biophysical
Chemistry
Miki Hasegawa (Japan), Inorganic Chemistry
Nikolay Nifantiev (Russia), Organic and Biomolecular
Chemistry

EX OFFICIO MEMBERS

Leah McEwen (USA), Committee on Publications and
Cheminformatics Data Standards, chair
Jürgen Stohner (Switzerland), Interdivisional Committee
on Terminology, Nomenclature and Symbols, chair
Hugh D. Burrows (Portugal), PAC Scientific Editor

DE GRUYTER

ABSTRACTED/INDEXED IN Baidu Scholar · Cabell's Whitelist · CABI (over 50 subsections) · Chemical Abstracts Service (CAS): CAplus · Chemical Abstracts Service (CAS) - SciFinder · Chimica · CNKI Scholar (China National Knowledge Infrastructure) · CNPIEC: cnpLINKer · Dimensions · EBSCO (relevant databases) · EBSCO Discovery Service · Ei Compendex · Engineering Village · Gale/Cengage · Genamics · JournalSeek · Google Scholar · Japan Science and Technology Agency (JST) · J-Gate · Journal Citation Reports/Science Edition · JournalGuide · JournalTOCs · KESLI-NDSL (Korean National Discovery for Science Leaders) · Microsoft Academic · MyScienceWork · Naver Academic · Naviga (Softweco) · Paperbase · Pirabase · Polymer Library · Primo Central (ExLibris) · ProQuest (relevant databases) · Publons · QOAM (Quality Open Access Market) · ReadCube · Reaxys · SCImago (SJR) · SCOPUS · Semantic Scholar · Sherpa/RoMEO · Summon (ProQuest) · TDNet · TEMA Technik und Management · Ulrich's Periodicals Directory/ulrichsweb · WanFang Data · Web of Science: Current Contents/Physical, Chemical and Earth Sciences; Science Citation Index; Science Citation Index Expanded · WorldCat (OCLC)

ISSN 0033-4545 · e-ISSN 1365-3075

All information regarding notes for contributors, subscriptions, Open access, back volumes and orders is available online at www.degruyter.com/pac

SCIENTIFIC EDITOR, CONFERENCE AND SPECIAL TOPIC PAPERS Prof. Hugh D. Burrows, Department of Chemistry, University of Coimbra, Coimbra, Portugal, e-mail: burrows@ci.uc.pt

EDITORS, IUPAC RECOMMENDATIONS AND TECHNICAL REPORTS Prof. Dr. Jürgen Stohner, Department of Life Sciences and Facility Management, Institute of Chemistry and Biotechnology, Zurich University of Applied Sciences, Waedenswil, Switzerland, e-mail: juergen.stohner@zhaw.ch
Prof. D. Brynn Hibbert, University of New South Wales, School of Chemistry, Sydney NSW 2052 Australia, e-mail: b.hibbert@unsw.edu.au

IUPAC SECRETARIAT PO Box 13757, Research Triangle Park, NC 27709-3757, USA; Tel.: +1 919-485-8700; Fax: +1 919-485-8706, e-mail: secretariat@iupac.org; Web site: www.iupac.org

PUBLISHER Walter de Gruyter GmbH, Berlin/Boston, Genthiner Straße 13, 10785 Berlin, Germany.

JOURNAL MANAGER Dr. Masha Dorogova, De Gruyter, Jarzabka str. 22/123, 05500 Piaseczno, Poland, Tel.: +48 798 238 728, e-mail: Masha.Dorogova@degruyter.com

RESPONSIBLE FOR ADVERTISEMENTS Markus Kügel, De Gruyter, Rosenheimer Str. 143, 81671 München, Germany. Tel.: +49 89 76 902-424, e-mail: anzeigen@degruyter.com.

TYPESETTING TNQ Technologies, Chennai, India

© 2021 Walter de Gruyter GmbH, Berlin/Boston, IUPAC

PRINTING Franz X. Stücker Druck und Verlag e.K., Ettenheim



Contents

Special topic paper

Lan Yuan, Zhaoyi Geng, Baoan Fan, Fen Guo and Chuang Han

State-of-the-art progress in tracking plasmon-mediated photoredox catalysis — 509

Invited papers

Elizabeth Ann Nalley

Leading by example — 525

Julian G. West

A blueprint for green chemists: lessons from nature for sustainable synthesis — 537

Fabio Aricò

Synthetic approaches to 2,5-bis(hydroxymethyl)furan (BHMF): a stable bio-based diol — 551

Conference papers

Virtual Conference on Chemistry and its Applications VCCA-2020

Aleksey E. Kuznetsov

Comparison of P- and As-core-modified porphyrins with the parental porphyrin: a computational study — 561

Li Cen Lim, Yee Ying Lim and Yee Siew Choong

Data curation to improve the pattern recognition performance of B-cell epitope prediction by support vector machine — 571

Nandini Savoo, Frederick P. Malan, Lydia Rhyman and Ponnadurai Ramasami

Molecular insights of metal–metal interactions in transition metal complexes using computational methods — 579

Prabhat Ranjan, Praveen K. Surolia and Tanmoy Chakraborty

Structure, electronic and optical properties of chalcopyrite-type nano-clusters $XFeY_2$ (X=Cu, Ag, Au; Y=S, Se, Te): a density functional theory study — 591

Zubaida Khalil and Muhammad Akhyar Farrukh

An efficient nanofiltration system containing mixture of rice husk ash and Fe/CeO_2-SiO_2 nanocomposite for the removal of azo dye and pesticide — 607

Sutopo Hadi, Sri Lestari, Tati Suhartati, Hardoko Insan Qudus, Mita Rilyanti, Dian Herasari and Yandri Yandri

Synthesis and comparative study on the antibacterial activity organotin(IV) 3-hydroxybenzoate compounds — 623

IUPAC Technical Report

Adriaan M. H. van der Veen, Juris Meija, Antonio Possolo and David Brynn Hibbert

Interpretation and use of standard atomic weights (IUPAC Technical Report) — 629