

CROATICA CT HEMICA

From Conceptual to Computational Chemistry and Back

*Festschrift in honour of
Professor Zvonimir Maksić*



GENERAL INSTRUCTIONS TO AUTHORS

Croatica Chemica Acta (CCA) is an international journal devoted to the publication of papers from all fields of chemistry. Four issues are published annually. Contributions should be written in English; an abstract (translated) in Croatian is added.

CCA publishes *Original scientific papers, Notes, Preliminary communications, Authors' reviews, Reviews, Feature articles, Conference papers, Essays* and *Data bank contributions*. In the appendix, the Journal publishes *Letters to the Editor, Book reviews, Obituaries* and the Croatian Chemical Society news.

Original scientific papers report unpublished results of original research. The papers have to contain all the necessary information to enable reproducibility of the described work.

Notes report unpublished results of short, but completed, original research or describe original laboratory techniques (methods, apparatus, etc.). *Notes* should not exceed 1000 words.

Preliminary communications report unpublished preliminary results of original research that require prompt publication.

Authors' reviews are concise and critical surveys of the author's current research field. The author's contribution should be compared to the data (results, information) provided by other scientists in the same field.

Reviews are concise and critical surveys of a specific research field, providing the reader with up-to-date information on current developments and trends. As a rule, reviews are written upon invitation from the Editor.

Feature articles are concise and critical reviews of a current topic, pointing to trends and controversies in the field. They should be understandable to non-specialists. Feature articles are written upon invitation from the Editorial Board and should not exceed 20 typewritten pages.

Conference papers should be reported at a congress, symposium or summer school prior to submission to the Journal. Conference papers are submitted by the Organizing Committee.

Essays report *curricula vitae* of the important Croatian chemists and accounts of the history of chemistry.

Data bank contributions contain new chemical and physical data in order to make them available for subsequent scientific interpretation and various practical uses.

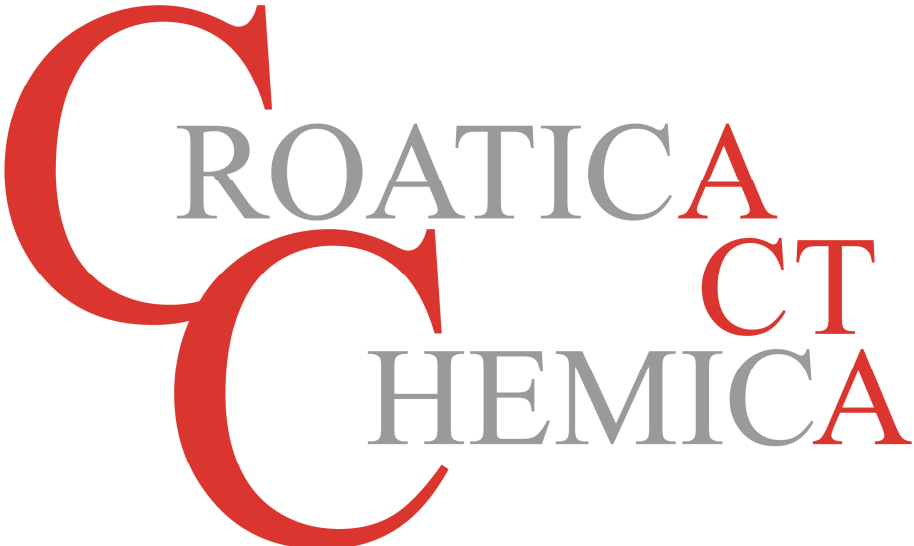
Letters to the Editor are a medium for expression of scientific opinions or exchange of different views concerning the material published in CCA.

All contributions are evaluated according to the criteria of originality and quality of their scientific content. *Original scientific papers, Notes* and *Preliminary communications* are sent to two referees, *Feature articles* and *Conference papers* to one, and *Authors' reviews, Reviews, Essays* and *Data bank contributions* to three. Only papers with favourable reports are accepted for publication.

Detailed *Instructions to Authors* are printed in the first issue of each volume and may be found on the web page <http://public.carnet.hr/ccaaa>

Cover page: The logo represents the coat-of-arms of the Croatian Chemical Society (Hrvatsko kemijsko društvo, HKD) established in 1926.

Published by the Croatian Chemical Society



CROATICA
ACT
HEMICA

Special Issue

Guest Editors

Davor Margetić

Robert Vianello

Croatica Chemica Acta is indexed in Chemical Abstracts Plus (CAPlus),
Science Citation Index (SCI), Science Citation Index Expanded (SCIE),
Current Contents – Physical, Chemical & Earth Sciences (CC),
SCOPUS, EBSCO – Academic Search Complete,
Directory of Open Access Journals (DOAJ),
Portal of Croatian Scientific Journals (HRČAK)

Croatica Chemica Acta is supported by the
Ministry of Science, Education and Sports of the Republic of Croatia

**ZAGREB
CROATIA
2009**

CROATICA CHEMICA ACTA

Published by the Croatian Chemical Society

Co-publishers

Faculty of Science, University of Zagreb
Horvatovac 102A, Zagreb, Croatia

Ruđer Bošković Institute
Bijenička c. 54, Zagreb, Croatia

Editor-in-Chief Nikola Kallay

Editors Ljerka Brečević
Tomica Hrenar
Predrag Novak

Assistant Editors Bono Lučić
Greta Prajdić

Technical Editors Miroslav Bajić
Ljerka Brečević
Zoran Kokan
Danijel Namjesnik
Greta Prajdić

Junior Editor Ozren Jović

Editorial Assistant Nada Trajkov

Honorary Editor Jean-Marie Lehn

Author of the Article Template Tomica Hrenar

EDITORIAL BOARD

Darko Babić
Goran Baranović
Mladen Biruš
Marina Cindrić
Vlasta Drevenkar

Milivoj Lovrić
Mirjana Metikoš
Kata Mlinarić-Majerski
Marija Šindler-Kulyk
Vladislav Tomišić

Hrvoj Vančik
Zorica Veksli
Ivana Weygand Đurašević
Dražen Vikić-Topić
Tomislav Živković

ADVISORY BOARD

F. H. Allen (UK)
A. M. Bond (Australia)
M. V. Diudea (Romania)
D. Hadži (Slovenia)
C. Giacobozzo (Italy)
R. Gleiter (Germany)
D. Grdenić (Croatia)
B. Kamenar (Croatia)
D. Keglević (Croatia)

D. J. Klein (USA)
M. Klessinger (Germany)
J. Kobe (Slovenia)
V. Kvasnička (Slovakia)
E. Matijević (USA)
A. de Meijere (Germany)
J. Mink (Hungary)
M. Randić (USA)
Ch. Rücker (Germany)

J. R. Sabin (USA)
Vl. Simeon (Croatia)
A. Simon (Germany)
D. Sunko (Croatia)
B. Stanovnik (Slovenia)
M. Tišler (Slovenia)
N. Trinajstić (Croatia)
J. Wang (USA)

Address of the Editorial Board

CROATICA CHEMICA ACTA

Horvatovac 102A, HR-10000 Zagreb, Croatia

Phone: +385 1 460 6163 Fax: +385 1 460 6131 E-mail: CCA@chem.pmf.hr