8th Conference of Young Chemists of Serbia

Book of Abstracts

29th October 2022 University of Belgrade, Faculty of Chemistry

СІР – Категоризација у публикацији

Народна библиотека Србије, Београд

54(048) 577.1(048) 60(048) 66.017/.018(048)

CONFERENCE of the Young Chemists of Serbia (8; 2022; Beograd) Book of abstracts / 8th Conference of the Young Chemists of Serbia, [Belgrade], 29th October 2022; [organized by Serbian Chemical Society [and] Serbian Young Chemists Club]; [editors Tamara Todorović ... [et al.]]. - Belgrade: Serbian Chemical Society: Serbian Young Chemists Club, 2022 (Belgrade: Development and Research Centre of Graphic Engineering Faculty of Technology and Metallurgy). - 150 str.: ilustr. + 24 cm Tiraž 20. - Bibliografija uz većinu apstrakata. - Registar. ISBN 978-86-7132-080-1

- 1. Srpsko hemijsko društvo (Beograd) 2. Klub mladih hemičara Srbije (Beograd)
- а) Хемија Апстракти b) Биохемија Апстракти c) Биотехнологија Апстракти d) Наука о материјалима Апстракти

COBISS.SR-ID 78648585

8th Conference of Young Chemists of Serbia

Belgrade, 29th October 2022

Book of Abstracts

Published and organized by

Serbian Chemical Society and Serbian Young Chemists' Club

Karnegijeva 4/III, 11000 Belgrade, Serbia

Tel./fax: +381 11 3370 467; www.shd.org.rs; office@shd.org.rs

Publisher

Dušan SLADIĆ, president of Serbian Chemical Society

Editors

Jelena MILOVANOVIĆ Jelena KESIĆ
Marko RODIĆ Mila LAZOVIĆ
Vuk FILIPOVIĆ Mihajlo JAKANOVSKI

Života SELAKOVIĆ

Page Layout and Design

Vuk FILIPOVIĆ Mila LAZOVIĆ

Jelena KESIĆ Mihajlo JAKANOVSKI

Circulation 20 copies

ISBN 978-86-7132-080-1

Printing

Development and Research Centre of Graphic Engineering

Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

Scientific Committee

Dr. Jelena Milovanović – University of Belgrade, Institute of molecular genetics and genetic engineering

Dr. Marko Rodić – University of Novi Sad, Faculty of Sciences

Dr. Vuk Filipović – University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia

Dr. Života Selaković – University of Belgrade, Faculty of Chemistry

Organizing Committee

Jelena Kesić – University of Novi Sad, Faculty of Sciences

Mila Lazović - Innovative Centre of the Faculty of Chemistry, Belgrade

Mihajlo Jakanovski - Innovative Centre of the Faculty of Chemistry, Belgrade

European Young Chemists' Network

Dr. Maximillian Menche, chair of the EYCN

Magnetic properties of altan-[n]annulenes

<u>Slađana Đorđević</u>¹, Slavko Radenković¹

¹ University of Kragujevac, Faculty of Science, Kragujevac, Serbia

The altanisation strategy is applied to [n]annulenes to give *altan*-[n]annulenes. In particular, *altan*-[24]annulene and *altan*-[30]annulene were examined in this study. These macrocyclic systems show unique optical, electrochemical, and magnetic properties. The structure of the studied molecules can be rationalized by means of an annulene-within-an-annulene model. The pseudo- π method for current density calculations was performed. In *altan*-[24]annulene, both annulene subunits sustain diatropic (aromatic) character in singlet and triplet states. On the other side, in *altan*-[30]annulene the outer ring sustain paratropic (antiaromatic) currents, but the inner ring sustain diatropic currents in the singlet state, but in the triplet state, both subunits sustain diatropic currents. Calculated *ef* values confirmed more intensive circulations in sixmembered rings than in five-membered rings.



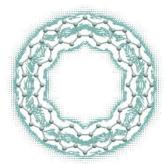


Figure 1. Maps of pseudo- π currents of altan-[30] annulene in singlet (left) and triplet state (right)

References

- 1. M. Piccardo, A. Soncini, P. Fowler, G. Monaco, R. Zanasi, *Phys. Chem. Chem. Phys.* **2020**, 22, 5476.
- 2. C. Liu et al, Chem, 2018, 4, 1586.

Acknowledgments

This work was supported by the Serbian Ministry of Education, Science and Technological Development, Serbia (Agreement No. 451-03-68/2022-14/200122).