

Srpsko hemijsko društvo



Serbian Chemical Society

**57. savetovanje
Srpskog hemijskog društva**

**KRATKI IZVODI
RADOVA
KNJIGA RADOVA**

**57th Meeting of
the Serbian Chemical Society**

**Book of Abstracts
Proceedings**

**Kragujevac 18. i 19. juni 2021.
Kragujevac, Serbia, June 18-19, 2021**

ISBN-978-86-7132-077-1

57. SAVETOVANJE SRPSKOG HEMIJSKOG DRUŠTVA

Kragujevac, 18. i 19. juni 2021.

KRATKI IZVODI RADOVA/KNJIGA RADOVA

57th MEETING OF THE SERBIAN CHEMICAL SOCIETY

Kragujevac, Serbia, June 18-19, 2021

BOOK OF ATRACTS/PROCEEDINGS

Izdaje / Published by

Srpsko hemijsko društvo / Serbian Chemical Society

Karnegijeva 4/III, 11000 Beograd, Srbija

tel./fax: +381 11 3370 467; www.shd.org.rs, E-mail: Office@shd.org.rs

Za izdavača/For Publisher

Dušan Sladić, predsednik Društva

Urednici/Editors, Dizajn korica, slog i kompjuterska obrada teksta/Cover Design, Page

Making and Computer Layout

prof. dr Snežana RAJKOVIĆ

Sladana ĐORĐEVIĆ

Snežana RADISAVLJEVIĆ

Milica MEĐEDOVIĆ

Tina ANDREJEVIĆ

OnLine publikacija/OnLine publication

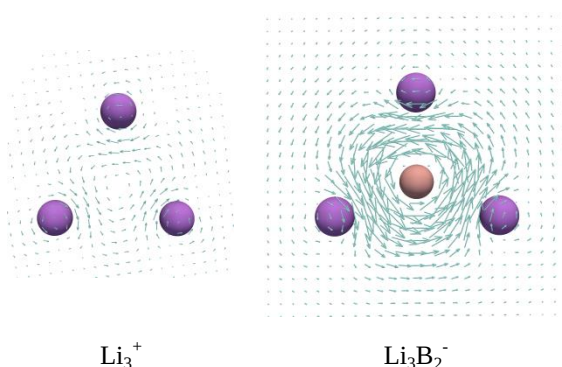
ISBN-978-86-7132-077-1

Podešavanje magnetno indukovanih gustina struja u Li klasterima

Sladana Đorđević, Slavko Radenković

Prirodno-matematički fakultet, Univerzitet u Kragujevcu, Radoja Domanovića 12, 34000 Kragujevac

Poznato je da monociklični Li_3^+ i Li_4^{2+} klasteri nisu aromatični. U prisustvu spoljašnjeg magnetnog polja, ovi klasteri pokazuju veoma slabe globalne gustine struja. U ovom radu je pokazano da uvođenje B_2^{2-} jedinice u ove sisteme daje klaster Li_3B_2^- i Li_4B_2 , koji se sastoje iz Li_3/Li_4 prstena između dva atoma bora. Pronađeno je da strukture Li_3/Li_4 u Li_3B_2^- i Li_4B_2 podsećaju na monociklične Li_3^+ i Li_4^{2+} klaster. Sa druge strane, magnetno indukovane gustine struje u Li_3B_2^- i Li_4B_2 , dobijene na M06-2X/CTOCD-DZ/def2-TZVP nivou teorije, suprotno od Li_3^+ i Li_4^{2+} , pokazuju izrazito diatropni karakter. Dobijene gustine struja se mogu direktno povezati sa elektronskom strukturom klastera preko analize virtuelnih prelaza iz popunjenih u nepopunjene molekulske orbitale.



Modulating the magnetically induced current density in monocyclic Li clusters

Sladana Đorđević, Slavko Radenković

Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac

It is known that the monocyclic Li_3^+ and Li_4^{2+} clusters are non-aromatic. In the presence of an external magnetic field these clusters show negligibly weak global current densities. In this work we showed that introduction of the B_2^{2-} unit in these systems resulted in stable Li_3B_2^- and Li_4B_2 clusters which consist of Li_3/Li_4 rings sandwiched by two boron atoms. We found that the Li_3/Li_4 rings in Li_3B_2^- and Li_4B_2 remarkably resemble the monocyclic Li_3^+ and Li_4^{2+} clusters. On the other hand, the magnetically induced current densities obtained at the M06-2X/CTOCD-DZ/def2-TZVP level of theory showed that in contrast to Li_3^+ and Li_4^{2+} , the Li_3B_2^- and Li_4B_2 clusters sustain a strong diatropic current density. The observed current densities in the studied clusters can be directly related to their electronic structure by analysing occupied-to-virtual orbital transitions.

Acknowledgement: This work was supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-9/2021-14/200122).