

Alkyltitanium ate complexes generated from alkylmagnesium halides and titanium TADDOLate : NMR and computational study

Kananovich, Dzmitry; Adamson, Jasper; **Osadchuk, Irina**; **Kudrjašova, Marina**; **Lopp, Margus** Balticum Organicum Syntheticum : 3-6 July 2016, Riga, Latvia : program and abstracts 2016 / p. 84 : ill http://www.boschem.eu/public/BOS2016/BOS-2016_Anstract-Book_Final.pdf

Anharmonic vibrational spectrum and experimental matrix isolation study of thioformic acid conformers-potential candidates for molecular cloud and solar system observations?

Lignell, A.; **Osadchuk, Irina**; Rasanen, M.; Lundell, J. The astrophysical journal 2021 / 7 p. : ill <https://doi.org/10.3847/1538-4357/ac06d0>
[Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Benchmarking computational methods and influence of guest conformation on chirogenesis in zinc porphyrin complexes

Osadchuk, Irina; **Borovkov, Victor**; **Aav, Riina**; Clot, Eric Physical chemistry chemical physics 2020 / p. 11025–11037
<https://doi.org/10.1039/D0CP00965B> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Challenges in mechanistic investigation of a flexible aminocatalyst as demonstrated through enamine formation

Osadchuk, Irina; **Kanger, Tõnis** ChemistryOpen 2025 / art. 2500116 <https://doi.org/10.1002/open.202500116> <https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/open.202500116>

Chirogenesis in Zinc porphyrins : theoretical evaluation of electronic transitions, controlling structural factors and axial ligation

Osadchuk, Irina; **Aav, Riina**; **Borovkov, Victor**; Clot, Eric ChemPhysChem 2021 / p. 1817–1833 : ill
<https://doi.org/10.1002/cphc.202100345> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Complexes of HXeY with HX (Y, X = F, Cl, Br, I) : symmetry-adapted perturbation theory study and anharmonic vibrational analysis

Dzieciol, Bartosz; **Osadchuk, Irina**; Cukras, Janusz; Lundell, Jan Molecules 2023 / art. 5148 <https://doi.org/10.3390/molecules28135148>
[Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Controlling chirogenic effects in porphyrin based supramolecular systems: theoretical analysis versus experimental observations

Osadchuk, Irina; **Luts, Hanna-Eliisa**; **Zahharova, Aleksandra**; **Tamm, Toomas**; **Borovkov, Victor** ChemPhysChem 2024 / art. e202400104 <https://doi.org/10.1002/cphc.202400104> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

ECD spectra of porphyrin complexes using TD-DFT

Osadchuk, Irina EUCMOS2023 : Abstract book 2023 / p. 42
https://jyx.jyu.fi/bitstream/handle/123456789/88819/EUCMOS2023_AbstractBook_FINAL_verkkoon.pdf?sequence=-1

Host-guest complexes of 2-aminocyclohexyl thioureas and zinc porphyrins: chiroptic properties and binding mechanism

Konrad, Nele; **Menailava, Darya**; **Osadchuk, Irina**; **Aav, Riina**; **Borovkov, Victor**; **Kananovich, Dzmitry** GSFMT Scientific Conference 2020 : Tallinn, February 4-5, 2020 : abstracts 2020 / p. 44 <http://fmtdk.ut.ee/wp-content/uploads/2020/01/GSFMT2020.pdf>

How different geometrical factors influence on ECD spectra of porphyrin-based supramolecules

Osadchuk, Irina 8th international conference on vibrational optical activity (VOA8) : book of abstracts 2024 / p. 76
https://www.mertenlab.de/wp-content/uploads/2024/08/VOA8_book_of_abstracts.pdf

Importance of molecular symmetry for enantiomeric excess recognition by NMR

Norvaiša, Karolis; O'Brien, John E.; **Osadchuk, Irina**; Twamley, Brendan; **Borovkov, Victor**; Senge, Mathias O. Chemical communications 2022 / p. 5423-5426 <https://doi.org/10.1039/D2CC01319C> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Induced circular dichroism in zinc porphyrin complexes

Osadchuk, Irina; **Aav, Riina**; Clot, Eric 1st International Conference on Noncovalent Interactions (ICNI 2019), 2-6 September, 2019 : program 2019 / poster 31, p. 34 https://icni2019.eventos.chemistry.pt/images/conference_program.pdf

Influence of activated carbon on ozonation of phenolic wastewater

Järvik, Oliver; **Saarik, Vardo**; **Osadchuk, Irina**; **Viiroja, Andres**; **Kamenev, Inna** 20th IOA World Congress - 6th IUVA World Congress : Ozone and UV Leading-Edge Science and Technologies : Paris, France, 23-27 May 2011 : proceedings 2011 / p. VIII.2.11-1 - VIII.2.11-9

Iridium PCP pincer complexes in electrochemical CO₂ hydrogenation

Osadchuk, Irina; Ahlquist, Marten S. G. TÜ ja TTÜ doktorikool "Funktsionaalsed materjalid ja tehnoloogiad" : 04.-05. märts 2014, Tartu 2014 / [2] p. : ill

Isomers and conformers of complexes of Ti(OiPr)₄ with cuclopentane-1,2-dione : NMR study and DFT calculations
Osadchuk, Irina; Pehk, Tõnis; Paju, Anne; Lopp, Margus; Öeren, Mario; Tamm, Toomas International journal of quantum chemistry 2014 / p. 1012-1018 : ill <https://doi.org/10.1002/qua.24619> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Mono-tsinkporfüriinide CD spektrite arvutuslik simuleerimine

Osadchuk, Irina XXXIV Eesti keemiapäevad : 100. aastapäeva teaduskonverentsi teesid 2019 / lk. 33 : ill https://www.ester.ee/record=b1580289*est

Reduced state of iridium PCP pincer complexes in electrochemical CO₂ hydrogenation

Osadchuk, Irina; Tamm, Toomas; Ahlquist, Marten S. G. ACS catalysis 2016 / p. 3834-3839 : ill <https://doi.org/10.1021/acscatal.6b01233> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Structures and catalytic properties of titanium and iridium based complexes = Titaani ja iriidiumi komplekside struktuur ja katalüütilised omadused

Osadchuk, Irina 2017 <https://digi.lib.ttu.ee/i/?7624> https://www.ester.ee/record=b4685981*est

Supramolecular chirogenesis in a sterically hindered Porphyrin : a critical theoretical analysis

Osadchuk, Irina; Luts, Hanna-Eliisa; Norvaiša, Karolis; Borovkov, Victor; Senge, Mathias O. Chemistry : a European journal 2023 / art. e202301408 <https://doi.org/10.1002/chem.202301408>

Supramolecular chirogenesis in a sterically hindered porphyrin: a critical theoretical analysis

Osadchuk, Irina; Luts, Hanna-Eliisa; Norvaiša, Karolis; Borovkov, Victor; Senge, Mathias O. Chemistry : a European journal 2023 / art. e202302275 <https://doi.org/10.1002/chem.202302275> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Supramolecular Chirogenesis in bis-porphyrin: crystallographic structure and CD spectra for a complex with a chiral guanidine derivative

Osadchuk, Irina; Konrad, Nele; Truong, Khai-Nghi; Rissanen, Kari; Clot, Eric; Aav, Riina; Kananovich, Dzmitry; Borovkov, Victor Symmetry 2021 / 14 p. : ill <https://doi.org/10.3390/sym13020275> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Supramolecular Chirogenesis in bis-porphyrin: crystallographic structure and CD spectra for a complex with a chiral guanidine derivative

Osadchuk, Irina; Konrad, Nele; Truong, Khai-Nghi; Aav, Riina; Kananovich, Dzmitry; Borovkov, Victor Chiral Auxiliaries and Chirogenesis II 2021 / p. 83-96 <https://doi.org/10.3390/sym13020275> <https://doi.org/10.3390/books978-3-0365-1155-9>

Supramolecular chirogenesis in zinc porphyrins: complexation with enantiopure thiourea derivatives, binding studies and chirality transfer mechanism

Konrad, Nele; Meniailava, Darya; Osadchuk, Irina; Adamson, Jasper; Hasan, Mohammed; Clot, Eric; Aav, Riina; Borovkov, Victor; Kananovich, Dzmitry Journal of porphyrins and phthalocyanines 2020 <https://doi.org/10.1142/S108842461950192X> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Theoretical investigation of a parallel catalytic cycle in CO₂ hydrogenation by (PNP)IrH₃

Osadchuk, Irina; Tamm, Toomas; Ahlquist, Marten S. G. Organometallics 2015 / p. 4932-4940 : ill <https://doi.org/10.1021/acs.organomet.5b00448> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Theoretical rationalization of chirality sensors on the basis of mono- and bis-porphyrins : abstract

Osadchuk, Irina Proceedings of the CSAC2021 : 1st International Electronic Conference on Chemical Sensors and Analytical Chemistry, 1–15 July 2021, MDPI: Basel, Switzerland : online 2021 / 1 p <https://doi.org/10.3390/CSAC2021-10550>

Thiourea organocatalysts as emerging chiral pollutants : en route to porphyrin-based (chir)optical sensing

Konrad, Nele; Horetski, Matvey; Sihtmäe, Mariliis; Osadchuk, Irina; Senge, Mathias O.; Borovkov, Victor; Aav, Riina; Kananovich, Dzmitry Chemosensors 2021 / art. 278 <https://doi.org/10.3390/chemosensors9100278> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Titaan-tsüklopentaandiooni-komplekside modell[e]erimine

Osadchuk, Irina; Tamm, Toomas XXXII Eesti Keemiapäevad : teaduskonverentsi teesid 2011 / lk. 69 : ill

Tsinkporfüriinide ja Takemoto katalüsaatori võõrustaja-külaline supramolekulaarse komplekside uurimine spektroskoopiliselt ja arvutuslikult

Konrad, Nele; Meniailava, D.; Osadchuk, Irina; Kananovich, Dzmitry XXXIV Eesti keemiapäevad : 100. aastapäeva teaduskonverentsi teesid 2019 / lk. 19 : ill