

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](#)

Behavior of Estonian kukersite kerogen in molecular mechanical force field

Lille, Ülo Oil shale 2004 / 2, p. 99-114 : ill https://artiklid.elnet.ee/record=b1015766*est

Biophysical studies of the amyloid beta-peptide : interactions with metal ions and small molecules

Wärmländer, Sebastian K.T.S.; Tiiman, Ann; Abelein, Axel Chembiochem : a European journal of chemical biology 2013 / p. 1692-1704 : ill <https://doi.org/10.1002/cbic.201300262> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Chirogenesis in Chemical Science

2023 <https://doi.org/10.1142/12915> https://www.ester.ee/record=b5748359*est

Computational study of cyclohexylhemicucurbiturils = Tsükloheksüülhemikukurbituriilide arvutuskeemiline modelleerimine

Öeren, Mario 2015 https://www.ester.ee/record=b4522693*est

Correlation queries for mass spectrometry imaging

Suits, Frank; Fehniger, Thomas Edward; Végvári, Ákos; Marko-Varga, György; Horvatovich, Peter Analytical Chemistry 2013 / p. 4398 - 4404 <https://doi.org/10.1021/ac303658t> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Crystallographic study of cyclohexanohemicucurbit[n]urils and their complexes

Kaabel, Sandra; Trunin, Madli; Topic, Filip; Rissanen, Kari; Aav, Riina ECS3 book of abstracts : Bol, Croatia, 25 Sept. - 02 Oct., 2016 2016 / p. 30 : ill http://ecs3.ecanews.org/PROGRAMME_files/ECS3_Book%20of%20Abstracts_z_v5.pdf

Design of heterobivalent molecules and their applications in chemical biology and materials science = Heterobivalentsete molekulide disain ning nende rakendused keemilises bioloogias ja materjaliteaduses

Bhadoria, Rohit 2020 <https://digikogu.taltech.ee/et/Item/1b7c1e2b-17e6-472e-a643-1e5cb9ea3929>

The development of surface imprinted thin films for immunoglobulin G molecular recognition

Boroznjak, Roman; Tretjakov, Aleksei; Reut, Jekaterina; Söritski, Vitali; Öpik, Andres MIP 2012 : 7th International Conference on Molecularly Imprinted Polymers Science and Technology : book of abstracts 2012 / p. 205

Elu võimalikkusest Internetis

Vilu, Raivo Biotoopia : Bioloogia. Tehnoloogia. Utopia. : Sorose Kaasaegse Kunsti Eesti Keskuse 3. aastanäitus, 22. november - 17. detsember 1995 1996 / 2 lk.: ill

Enhancing binding properties of imprinted polymers for the detection of small molecules

Ayankojo, Akinrinade George; Reut, Jekaterina; Öpik, Andres; Tretjakov, Aleksei; Söritski, Vitali Proceedings of the Estonian Academy of Sciences 2018 / p. 138-146 : ill <https://doi.org/10.3176/proc.2018.2.04> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Experimental determination of the interaction potential between a helium atom and the interior surface of a C60 fullerene molecule

Bacanu, George Razvan; Jafari, Tanzeeha; Aouane, Mohamed; Rantaharju, Jyrki; Walkey, Mark; Hoffman, Gabriela; Shugai, Anna; Nagel, Urmas; Jimenez-Ruiz, Monica; Horsewill, Anthony J.; Rols, Stephane; Rõõm, Toomas; Whitby, Richard J.; Levitt, Malcolm H. The Journal of chemical physics 2021 / art. 144302 <https://doi.org/10.1063/5.0066817>

Fast atomic charge calculation for implementation into a polarizable force field and application to an ion channel protein

Witter, Raiker; Möllhoff, Margit; Koch, Frank-Thomas; Sternberg, Ulrich Journal of chemistry 2015 / p. 1-14 : ill <https://doi.org/10.1155/2015/908204> [Journal metrics at Scopus](#) [Article at Scopus](#) [Article at WOS](#)

Fluorene- and fluorenone-based molecules as electron-transporting SAMs for photovoltaic devices

Svirskaitė, Lauryna Monika; Kasparavicius, Ernestas; Steponaitis, Matas; Grzibovskis, Raitis; Franckevicius, Marius; Katerski, Atanas; Naujokaitis, Amas; Karazhanov, Smagul; Gopi, Sajeesh Vadakkedath; Aizstrauts, Arturs RSC advances 2024 / p. 14973-14981 <https://doi.org/10.1039/D4RA00964A> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Halogen and chalcogen polyhydrides

Luts, Hanna-Eliisa; Tamm, Toomas ICQC 2023 : International Congress of Quantum Chemistry : Book of Abstracts 2023 / p. PB48 <https://icqc2023.org/wp-content/uploads/BOA-27-6-v1.pdf>

Hemodialysis optical monitoring toward greener technology : a potential for water saving dialysis treatment

Leis, Liisi; Adoberg, Annika; Paats, Joosep; Holmar, Jana; Arund, Jürgen; Karai, Deniss; Luman, Merike; Pilt, Kristjan;

Taklaja, Paul; Tanner, Risto; Fridolin, Ivo 19th Nordic-Baltic Conference on Biomedical Engineering and Medical Physics : Proceedings of NBC 2023, June 12–14, 2023, Liepaja, Latvia 2023 / p. 162 - 171 https://doi.org/10.1007/978-3-031-37132-5_21
[Conference Proceedings at Scopus](#) [Article at Scopus](#)

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

Impacts of lubricating oils on rheology and chemical compatibility of asphalt binders

Teymourpour, Pouya; **Sillamäe, Sven**; Bahia, Hussain U. Road Materials and Pavement Design 2015 / p. 50 - 74
<https://doi.org/10.1080/14680629.2015.1030833> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Large azobenzene acrocycles : formation and detection by NMR and MS methods

Roithmeyer, Helena; **Uudsemaa, Merle**; Trummal, Aleksander; **Brük, Mari-Liis**; Krämer, Sebastian; **Reile, Indrek**; Rjabovs, Vitalijs; Palmi, Kirsti; **Rammo, Matt**; **Aav, Riina**; Kalenius, Elina; Adamson, Jasper Supramolecular Chemistry 2022 / p. 77-86
<https://doi.org/10.1080/10610278.2023.2230334> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Maristem - stem cells of marine/aquatic invertebrates : from basic research to innovative applications

Ballarin, Lorian; Rinkevich, Baruch; Bartscherer, Kestin; Bartscherer, Kestin; Cambier, Sebastien; Cammarata, Matteo; Domart-Coulon, Isabelle; Drobne, Damjana; Encinas, Juanma; Frank, Uri; Geneviere, Anne-Marie; Hobmayer, Bert; **Löhelaid, Helike**; Lyons, Daniel; Martinez, Pedro; Oliveri, Paola; Peric, Lorena; Piraino, Stefano; Ramšak, Andreja; Rakers, Sebastian; Rentzsch, Fabian; Rosner, Amalia; Silva, Tiago Henriques da; Somorjai, Idiko; Suleiman, Sherif; Coelho, Ana Varela Sustainability (Switzerland) 2018 / Art. 526 <https://doi.org/10.3390/su10020526> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Microbial cancer therapeutics : a promising approach

Diwan, Deepti; Cheng, Lei; **Usmani, Zeba**; Sharma, Minaxi; Holden, Nicola; Willoughby, Nicholas; Sangwan, Neelam; Baadhe, Rama Raju; Liu, Chenchen; Gupta, Vijai Kumar Seminars in Cancer Biology 2022 / p. 931 - 950
<https://doi.org/10.1016/j.semcancer.2021.05.003> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Microcanonical rate constant in case of intramolecular large amplitude vibrations

Metsala, Andrus 23rd Estonian Chemistry Days : abstracts of scientific conference 1997 / p. 92

Mikrokanooniline kiiruskonstant suureamplituudiliste molekulisise vönkumiste korral

Metsala, Andrus XXIII Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid 1997 / lk. 83

Mis on vesi?

Munter, Rein Mente et Manu 2022 / lk. 46-49 : ill https://www.ester.ee/record=b1242496*est

Mittestatistilised vinüülbromiidi molekulis

Metsala, Andrus XXVIII Eesti keemiapäevad : teaduskonverentsi ettekannete teesid = 28th Estonian Chemistry Days : abstracts of scientific conference 2002 / lk. 86

Modeling the toxicity of chemicals to Tetrahymena pyriformis using heuristic multilinear regression and heuristic back-propagation neural networks

Kahn, Iiris; Sild, Sulev; Maran, Uko Journal of chemical information and modeling 2007 / 6, p. 2271-2279
<https://pubs.acs.org/doi/10.1021/ci700231c>

Molecular dynamics simulations on PGLa using NMR orientational constraints

Sternberg, Ulrich; **Witter, Raiker** Journal of biomolecular NMR 2015 / p. 265-274 : ill <https://doi.org/10.1007/s10858-015-9983-y>
[Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Molekulid kuvariekraanil

Köstner, Ado Tehnika ja Tootmine 1990 / 4, lk. 21-23: ill

Molekulide püüdmine

Õpik, Andres Tarkade Klubi 2010 / erinumber, lk. 50

Molekulide XeOn (n=2-4) arvutused : kas ksenoonidoksiidi molekul võiks eksisteerida? = Calculations for XeOn (n=2-4): could the xenon dioxide molecule exist?

Tamm, Toomas; Pyykkö, P. XXV Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid = 25th Estonian Chemistry Days : abstracts of scientific conference 1999 / lk. 166

Multiple secondary interaction arrangement in the crystal structure of cis-dichlorobis(thiourea-S)-zinc(II)

Bombicz, Petra; Madarasz, Janos; **Krunks, Malle**; Niinistö, Lauri; Pokol, György Journal of coordination chemistry 2007 / 4, p. 457-464 <https://www.tandfonline.com/doi/abs/10.1080/00958970600873604>

Nanorobotid elusorganismis ja inimnaha liim - see on supramolekulaarne keemia

Aav, Riina Inseneeria 2015 / lk. 30-32 : ill https://artiklid.elnet.ee/record=b2741120*est

Neutraalsete molekulide superhappelisus ja superaluselisus

Koppel, I.; Burk, Peeter XVI Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid = 16th Estonian chemistry days : abstracts of scientific conference 1995 / lk. 54-57

New oxalix[4]arene carboxylate detects viologen in protic media

Peterson, Anna; Ludvig, Mari-Liis; Martõnova, Jevgenija; Kaabel, Sandra; Fomitšenko, Maria; Aav, Riina Supramolecular chemistry 2020 / p. 313–319 : ill <https://doi.org/10.1080/10610278.2019.1659269> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Oksakaliks[4]areeni derivaatide süntees

Ludvig, Mari-Liis; Peterson, Anna; Martõnova, Jevgenija; Aav, Riina; Adamson, Jasper XXXIV Eesti keemiapäevad : 100. aastapäeva teaduskonverentsi teesid 2019 / lk. 24 : ill

Omega-3 fatty acid and B12 vitamin content in Baltic algae

Luhila, Önnela; Paalme, Tiina; Tanilas, Kristel; Sarand, Inga Algal Research 2022 / Art. 102860

<https://doi.org/10.1016/j.algal.2022.102860> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

POS-648 medicines intake influences accuracy of the uremic retention molecules' optical monitoring in spent dialysate : the case of uremic toxin uric acid and paracetamol

Paats, Joosep; Adoberg, Annika; **Arund, Jürgen; Fridolin, Ivo; Holmar, Jana;** Leis, Liisi; **Pilt, Kristjan; Tanner, Risto; Uhlin, Nils Fredrik Arne; Luman, Merike** Kidney International Reports 2022 / p. S277-S278 : ill <https://doi.org/10.1016/j.ekir.2022.01.681>

QSAR of heterocyclic compounds in large descriptor spaces

Karelson, Mati; Dobchev, Dimitar Atanasov Advances in Heterocyclic Chemistry ; Vol. 120 2016 / p. 237 - 273

<https://doi.org/10.1016/bs.aihch.2016.03.006> [Article collection metrics at Scopus](#) [Article at Scopus](#) [Article collection metrics at WOS](#) [Article at WOS](#)

QSPR modelling of solubility of polyaromatic hydrocarbons and fullerene in 1-octanol and n-heptane

Martin, Dana; Maran, Uko; Sild, Sulev; **Karelson, Mati** Journal of physical chemistry B 2007 / 33, p. 9853-9857

<https://pubs.acs.org/doi/10.1021/jp071679x>

QSPR study of critical micelle concentration of anionic surfactants using computational molecular descriptors

Karitzky, Alan R.; Pacureanu, Liliana; Dobchev, Dimitar; **Karelson, Mati** Journal of chemical information and modeling 2007 / 3, p. 782-793 <https://pubs.acs.org/doi/10.1021/ci600462d>

Quantum dynamics of noble gas atoms and methane in the molecular cavity of fullerene : terahertz spectroscopy study =

Väärisgaasi aatomite ja metaani kvantdünaamika fullereeni molekulaarses õõnsuses : terahertsspektroskoopia uurimus

Jafari, Tanzeeha 2025 <https://digikogu.taltech.ee/et/Item/33879cfc-2e32-4b05-bdbc-86e033784086> <https://doi.org/10.23658/taltech.6/2025>

https://www.ester.ee/record=b5728363*est

Rein Munter: Vesi mäletab

Munter, Rein Tähtenduse Teejuhid 2021 / Lk. 9 <https://teejuhid.postimees.ee/7319813/rein-munter-vesi-maletab>

Sample plate modification for improvement of sensitivity in analysis of small molecules by MALDI-MS

Borissova, Maria; Vaher, Merike; Kaljurand, Mihkel IUPAC International Congress on Analytical Sciences 2011 : 22-26 May 2011, Kyoto, Japan 2011

Simulations of propane and butane gas sensor based on pristine armchair graphene nanoribbon

Rashid, Muhammad Haroon; Koel, Ants; Rang, Toomas IOP conference series : materials science and engineering 2018 / art.

012001, 8 p <https://doi.org/10.1088/1757-899X/362/1/012001> [Conference proceedings at Scopus](#) [Article at Scopus](#) [Article at WOS](#)

Squeezing formaldehyde into C60 fullerene

Vyas, Vijyesh K.; Bacanu, George Razvan; Soundararajan, Murari; Marsden, Elizabeth S.; **Jafari, Tanzeeha;** Shugai, Anna; Light, Mark E.; Nagel, Urmas; Rõõm, Toomas; Levitt, Malcolm H.; Whitby, Richard J. Nature Communications 2024 / art. 2515

<https://doi.org/10.1038/s41467-024-46886-5> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Supramolecular systems based on novel amphiphiles and a polymer : aggregation and selective solubilization

Gabdrakhmanov, Dinar; Samarkina, Darya; Krylova, Evgeniya; **Kapitanov, Illia; Karpichev, Yevgen** Journal of surfactants and

detergents 2019 / p. 865-874 : ill <https://doi.org/10.1002/jsde.12257> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Synthesis of chiral urea-based macrocycles and their application as molecular containers = Kiraalsete urea-põhiste molekulaarsete mahutite süntees ja rakendus

Mishra, Kamini Atindrakumar 2022 <https://doi.org/10.23658/taltech.20/2022> <https://digikogu.taltech.ee/et/Item/b07b0d8d-888b-420d-839e-a809b9d5cfce> https://www.ester.ee/record=b5500524*est

TalTechi keemikud segavad molekule nagu meisterkokad

Uusen, Kaire Trialoog 2025 <https://trialoog.taltech.ee/taltech-keemikud-segavad-molekule-nagu-meisterkokad/>

The antisymmetric stretching frequency of BO₂

Lomp, Peeter-Egil; Stepanov, N.; Simkin, V.; Dementjev, A. Eesti NSV Teaduste Akadeemia toimetised. Keemia = Proceedings of Academy of Sciences of the Estonian SSR. Chemistry = Известия Академии наук Эстонской ССР. Химия 1985 / lk. 231-234 https://www.ester.ee/record=b1264984*est <https://www.etera.ee/zoom/19206/view?page=1&p=separate&tool=info>

Theoretical investigation of the O-B-O → B-O-O rearrangement

Lomp, Peeter-Egil; Simkin, V.; Dementjev, A.; Stepanov, N. Eesti NSV Teaduste Akadeemia toimetised. Keemia = Proceedings of Academy of Sciences of the Estonian SSR. Chemistry = Известия Академии наук Эстонской ССР. Химия 1985 / lk. 235-236 https://www.ester.ee/record=b1264984*est <https://www.etera.ee/zoom/19206/view?page=1&p=separate&tool=info>

Two-photon voltmeter for measuring a molecular electric field

Rebane, Aleksander; Wicks, Geoffrey; Drobizhev, Mikhail; Cooper, Thomas; Trummal, Aleksander; **Uudsemaa, Merle** Angewandte Chemie - International Edition 2015 / p. 7582 - 7586 <https://doi.org/10.1002/anie.201502157> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Uudsed "keemilised ninad" aitavad keskkonda puhastada

Imeline Teadus 2019 / lk. 20 : fot https://www.ester.ee/record=b2747925*est

Uued asümmeetrilised reaktsioonid ja nende katalüsaatorid

Lopp, Margus; Paju, Anne; Kanger, Tõnis Mente et Manu 2004 / 9. märts, lk. 3 https://www.ester.ee/record=b1242496*est https://artiklid.elnet.ee/record=b1018852*est

Uureapõhised molekulaarsed mahutid

Aav, Riina Tallinna Tehnikaülikooli aastaraamat 2013 2014 / lk. 243-247 : ill

Veekriis ja vee elutähtis olemus

Munter, Rein Horisont 2020 / lk. 30-34 : ill https://www.ester.ee/record=b1072243*est

Vinyl phosphonates as photopharmacological agents : laser-induced cis-trans isomerization and butyrylcholinesterase activity

Bikbaeva, Gulia; Egorova, Anastasia; Sonin, Nikolai; Pilip, Anna; Kolesnikov, Ilya; Pankin, Dmitrii; **Boroznjak, Roman**; Manshina, Alina ChemPhotoChem 2023 / art. e202300131 <https://doi.org/10.1002/cptc.202300131> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Аналитическое применение донор-акцепторных комплексов кислородных соединений II

Lippmaa, Helle Сборник статей по химии и химической технологии. 13 1965 / с. 61-66 https://www.ester.ee/record=b2182034*est <https://digikogu.taltech.ee/et/Item/d4d94766-1dca-4956-8efe-f305fca83182>

Аналитическое применение донор-акцепторных комплексов кислородных соединений

Lippmaa, Helle Сборник статей по химии и химической технологии. 13 1965 / с. 43-56 https://www.ester.ee/record=b2182034*est <https://digikogu.taltech.ee/et/Item/d4d94766-1dca-4956-8efe-f305fca83182>

Изучение общей и парциальных упругостей паров водных растворов хлорозамещенных уксусных кислот в связи с вопросом об ассоциации молекул

Schmidt, Ludvig 1940

Исследование водородных связей в кристаллических молекулярных комплексах ε-капролактама - двухатомные фенолы 2 : 1 методом ИК-спектроскопии

Oja, Holger Синтез и применение поликонденсационных клеев. 2 1978 / с. 101-116 : илл https://www.ester.ee/record=b2191006*est <https://digikogu.taltech.ee/et/Item/b615a4dd-bb4c-4a80-888a-b13d1a4c52d3>