

A simplified open-shell solvation model

Uudsemaa, Merle; Tamm, Toomas Xth International Congress of Quantum Chemistry : July 20-26, 2003, Germany : program and abstracts 2003 / p. A51

Acid/base properties of some conformationally flexible organocatalysts

Uudsemaa, Merle; Kanger, Tõnis; Tamm, Toomas 13th ICQC International Congress of Quantum Chemistry : June 22-27, 2009, Helsinki, Finland : abstracts and program 2009 / p. 168

Calculation of hydration enthalpies of aqueous transition metal cations using two coordination shells and central ion substitution

Uudsemaa, Merle; Tamm, Toomas Chemical physics letters 2004 / 1/3, lk. 54-58 : ill
<https://www.sciencedirect.com/science/article/abs/pii/S0009261404016781>

Calculations of hydrated titanium ion complexes : structure and influence of the first two coordination spheres

Uudsemaa, Merle; Tamm, Toomas Chemical physics letters 2001 / p. 667-672
<https://www.sciencedirect.com/science/article/pii/S0009261401006170>

Density-functional theory calculations of aqueous redox potentials of fourth-period transition metals

Uudsemaa, Merle; Tamm, Toomas Journal of physical chemistry A 2003 / p. 9997-10003 : ill
<https://pubs.acs.org/doi/10.1021/jp0362741>

Enantioselective organocatalytic Michael addition of aldehydes to [beta]-nitrostyrenes

Laars, Marju; Ausmees, Kerti; Uudsemaa, Merle; Tamm, Toomas; Kanger, Tõnis; Lopp, Margus The journal of organic chemistry 2009 / p. 3772-3775 <https://pubs.acs.org/doi/full/10.1021/jo900322h>

Energetics of solvated transition metal complexes

Tamm, Toomas; Uudsemaa, Merle Xth International Congress of Quantum Chemistry : June 5-10, 2000, Menton France 2000 / p. B76

Hydration enthalpies and redox potentials from DFT calculations

Uudsemaa, Merle; Tamm, Toomas Exploring Modern Computational Chemistry 2002 / ? p

Inclusion of additional coordination sphere into cluster-model redox potential calculations

Uudsemaa, Merle; Tamm, Toomas AIP conference proceedings 2007 / 2, p. 495-499
<https://ui.adsabs.harvard.edu/abs/2007AIPC..963..495U/abstract>

Influence of protonation upon the conformations of biperidine, bismorpholine, and their derivatives

Uudsemaa, Merle; Laars, Marju; Kriis, Kadri; Tamm, Toomas; Lopp, Margus; Kanger, Tõnis Chemical physics letters 2009 / 1/3, p. 92-96 <https://www.sciencedirect.com/science/article/abs/pii/S0009261409001857>

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

Rõithmeyer, 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](#)

Matemaatika-loodusteaduskond : [tutvustus]

Anderson, Wally; Uudsemaa, Merle Mente et Manu 2005 / Uudistaja, lk. 6 : fot https://www.ester.ee/record=b1242496*est

Novel lipophilic fluorophores with highly acidity-dependent two-photon response

Rammo, Matt; Trummal, Aleksander; Uudsemaa, Merle; Pahapill, Jüri; Petritsenko, Katrin; Sildoja, Meelis-Mait; Stark, Charles William; Selberg, Sigrid; Leito, Ivo; Palmi, Kristi; Adamson, Jasper; Rebane, Aleksander Chemistry : a European journal 2022 / p. e202103707 <https://doi.org/10.1002/chem.202103707>

On-off-on control of molecular inversion symmetry via multi-stage protonation : elucidating vibronic laporte rule

Stark, Charles William; Rammo, Matt; Trummal, Aleksander; Uudsemaa, Merle; Pahapill, Jüri; Sildoja, Meelis-Mait; Tshepelevitsh, Sofija; Leito, Ivo; Young, David C.; Szymanski, Bartosz; Vakuliuk, Olena; Gryko, Daniel T.; Rebane, Aleksander Angewandte Chemie international edition 2022 / p. e202212581 <https://doi.org/10.1002/anie.202212581>

Parahydrogen hyperpolarized NMR detection of underivatized short oligopeptides

Reimets, Nele; Ausmees, Kerti; Vija, Sirje; Trummal, Aleksander; Uudsemaa, Merle; Reile, Indrek Analyst 2023 / p. 5407-5415 : ill
<https://doi.org/10.1039/d3an01345f> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

pKa calculation for monoprotonated biperidine, bismorpholine and their derivatives in H₂O and MeCN

Uudsemaa, Merle; Kanger, Tõnis; Lopp, Margus; Tamm, Toomas Chemical physics letters 2010 / p. 83-86
<https://www.sciencedirect.com/science/article/pii/S000926140901519X>

Quantum-chemical modeling of solvated first row transition metal ions = Solvateeritud üleminekumetalli-ioonide kvantkeemiline modelleerimine

Uudsemaa, Merle 2006 https://www.ester.ee/record=b2146117*est

Redox potentials from DFT calculations

Uudsemaa, Merle; Tamm, Toomas XIth International Congress of Quantum Chemistry : May 21-26, 2006, Kyoto, Japan : program and abstract 2006 / p. B075

Solution- and gas-phase study of binding of ammonium and bisammonium hydrocarbons to oxalix[4]arene carboxylate

Cowart, Anna; Brük, Mari-Liis; Žoglo, Nikita; Roithmeyer, Helena; Uudsemaa, Merle; Trummal, Aleksander; Selke, Kaspar; Aav, Riina; Kalenius, Elina; Adamson, Jasper RSC advances 2023 / p. 1041–1048 : ill <https://doi.org/10.1039/d2ra07614d>

Spin state of Co²⁺, Co³⁺ and Ni³⁺ ions on solution

Uudsemaa, Merle; Tamm, Toomas 11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics 2005 / p. P225

Titaani akvakomplekside kvantkeemilised arvutused

Uudsemaa, Merle; Tamm, Toomas XXVI Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid = 26th Estonian Chemistry Days : abstracts of scientific conference 2000 / lk. 150

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](#)